Workshop: Research Needs for Material Mixing at Extremes

La Fonda Hotel, Santa Fe, New Mexico
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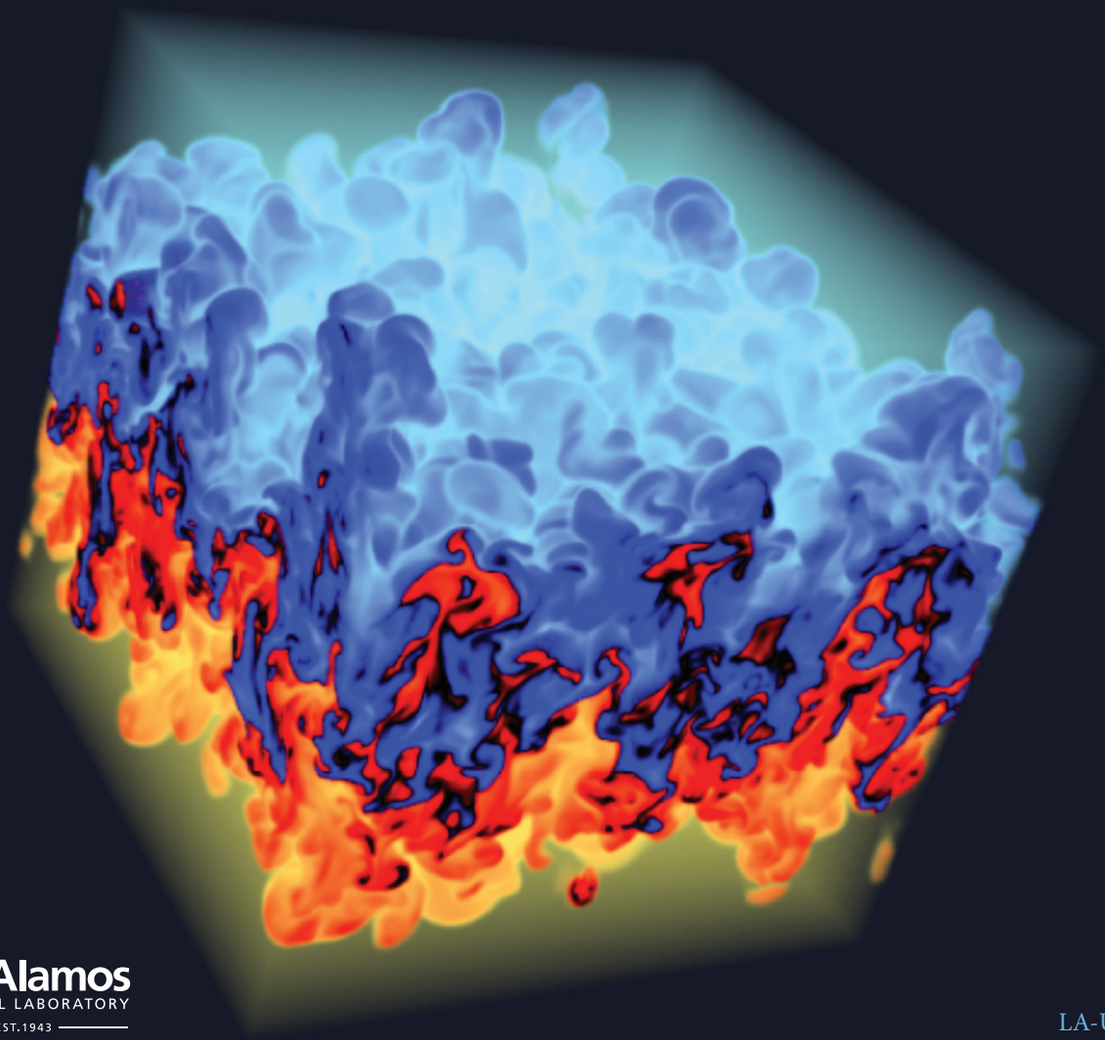

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1. Executive Summary

Material Mixing underpins modern technologies and science that range from relatively benign and slow effects in climate, to reactive and fast energy release in Inertial Confinement Fusion. Stating such a broad range can miss the diversity of applications in between that include combustion, supersonic flows, explosions, spray development, and environmental flows. At the heart of the present material mixing workshop is fluid flow, and its ability to mix materials often (but not always) by turbulence. Despite the number of modern applications, the lack of knowledge and progress toward the full understanding of material mixing processes motivated the present workshop, with a goal to map out priority research directions, and cross-cutting issues. Indeed, the charge to the workshop was stated as:

> *"The last 25 years has seen substantial progress with understanding material mixing in low energy environments, particularly with the development of high fidelity experimental multi-probe diagnostics, direct numerical simulations, and science based theories and mathematical models. We now need to move such advances to the high energy environment with a goal to increase our understanding and predictability, and raise our confidence in scientifically informed decision making. Thus, this workshop is charged to look to the future (~ 15 years), and explore opportunities to advance our current understanding of material mixing in extreme conditions."*

With this charge in-hand the workshop has proposed 18 priority research directions (4 Theory, 4 Simulation, and 10 Experiments, in sections 3.3, 4.3, and 5.3, respectively) and identified various capability needs and capability gaps. The future then holds promise for improved fundamental understanding of material mixing, and also improved predictive capability and associated technological performance. Thus, this workshop envisages a set of innovative experiments driven by a suite of theoretical questions and simulation needs and requirements. Such a route demands the development of new facilities, diagnostics, numerical analysis and methods, and new theories. This "co-design" of experiment/computation/theory is the hallmark of successful fluid research in general, and a necessity for material mixing.

This report describes the outcomes from the workshop, but is not planned to be the only reporting means by which the deliberations and recommendations from the workshop will be disseminated; also planned is an archival journal paper in the ASME *Journal of Fluids Engineering*, and a follow-up decadal study, as a means to further widen the platform of future developments for material mixing.

The workshop organizer, Dr. Malcolm Andrews of group XCP-4 at Los Alamos National Laboratory, takes this opportunity to thank the participants for a very productive workshop, his co-organizers, and special thanks to the sponsors, in particular, the MaRIE (Matter-Radiation Interactions in Extremes) team at Los Alamos, the CoMuEx (Center of Mixing Under Extreme Conditions), and the ASME.

2. Introduction

This report describes the work done during, and results from, the "Research Needs for Material Mixing at Extremes" workshop held at the La Fonda Hotel in Santa Fe, New Mexico, January 9–12, 2011. The workshop was organized around three interrelated themes/panels, namely, Theory/Modeling, Simulations/Predictions, and Experiments/Diagnostics and their application to material mixing. With this organization the goals of the workshop were to:

- Raise the general awareness of material mixing problems in extreme conditions.
- Peer into the future (15 years) for theory/modeling, simulation/predictions, and experiments/diagnostics in relation to material mixing.
- Identify priority research directions, capability opportunities, and projected capability needs.
- Produce a report, a peer reviewed journal paper, and a proposal for a decadal study.

In preparation for the workshop, a set of preliminary questions for consideration by each of the panels was distributed to the participants (see Appendix A) and served to initiate discussion during breakout sessions. The workshop agenda may be found in Appendix B. The workshop was structured as three invited plenary talks on the first morning that addressed fundamentals, integrated problems, and an illustrative overarching application. This was followed by breakout panels to consider pre-determined questions and address the goals of the workshop, particularly priority research directions, capability opportunities, and capability gaps. The panels consisted of different sets of participants, and, as a consequence, the reports from the panels have overlap. For completeness, and because the overlapping discussions did differ, the individual reports of the panels are given in the following chapters without editing the overlap. The first day was concluded with dinner and an after-dinner speaker, Dr. Michael Dunne from Lawrence Livermore National Laboratory, who spoke on "why controlling mix could enable LIFE (Laser Inertial Fusion Energy)". The second day continued the breakout panels but with more detailed discussion, cross-panel interaction, and panel out-briefs. The morning of the third day was devoted to writing this report and follow-up assignments.

Thus, this report is structured to reflect the discussion and address the goals of the workshop. In particular, each panel discussion is summarized next in sections 3, 4 and 5, starting with Theory and Modeling, followed by Predictions and Simulations, and closing with Experiments and Diagnostics. Overlapping discussions have been kept in the spirit of the workshop, and to provide alternative views of similar topics. This order is chosen to capture the flow from theory to experiment, i.e., the "driver" to the "engine". The report closes with a summary of priority research directions, references, and Appendices that include the pre-workshop questions, agenda, and, where possible, details of possible experiments.

3. Theory and Modeling (O. Schilling and D. Pullin)

3.1 Summary

The theory/modeling panel discussed the principal challenges associated with predictive modeling of complex hydrodynamics and turbulent mixing induced primarily by acceleration-, shock- and shear-driven flows, i.e., Rayleigh–Taylor, Richtmyer–Meshkov and Kelvin–Helmholtz instabilities (Sharp, 1984; Brouillette, 2002; Drazin and Reid, 2004). Turbulent flows and mixing driven by these instabilities are of fundamental as well as applied interest to a wide range of low- and high-energy-density phenomena. Relevant examples at low-energy-density include the ocean mixed layer and stratified turbulence, atmospheric inversion, atomization of droplets and sprays, multiphase flows, supersonic combustion, and chemically-reacting flows. Relevant examples at high-energy-density (HED) include inertial confinement fusion (ICF) and astrophysical flows such as supernovae and molecular clouds in the interstellar medium.

Rayleigh–Taylor instability results from misaligned density and pressure gradients satisfying $\nabla\rho\cdot\nabla p<0$ when a lighter fluid accelerates a heavier fluid separated by a perturbed interface. Richtmyer–Meshkov instability occurs when a shock traverses a perturbed interface, depositing vorticity on the interface. Baroclinic vorticity production $\nabla\rho\times\nabla p/\rho^2$ is a key process in both of these instabilities. An important process associated with Richtmyer–Meshkov instability is reshock of the evolving mixing layer, which baroclinically deposits additional vorticity and compresses the layer. Kelvin-Helmholtz instability is driven by velocity shear, producing rollups with “mushroom” caps primarily on the spikes of the heavier fluid in Rayleigh–Taylor and Richtmyer–Meshkov instability.

Hydrodynamic instability-induced turbulent material mixing has a number of distinct features compared to more typical “canonical” turbulent flows, which include but are not limited to:

1. Anisotropy and inhomogeneity from initial conditions, geometry, and preferred flow direction (e.g., time-varying accelerations or shocks).
2. Material discontinuities and shocks.
3. Baroclinic effects due to vorticity production near interfaces.
4. Multifluid shear and mixing (rather than single-fluid shear and mixing of a scalar field).
5. Varying density, locally strong compressibility, and nonequilibrium (e.g., during reshock).
6. Transitional and unsteady flow.
7. Flows with a very wide range of Reynolds (Re), Atwood (At), Schmidt (Sc), Mach (Ma) and other dimensionless numbers.
8. Mixture properties (equation of state, transport coefficients, etc.).
9. Chemical or thermonuclear reactions among species.
10. Elastoplastic and material strength effects.
11. The plasma state with radiation transport coupled to hydrodynamics in HED applications.

Within the context of the flow complexity summarized above, the topics considered by the panel included (and discussed in section 3.2 below) how to more precisely define predictive modeling for this class of flows, examples of limitations or failures of classical models (including numerical simulation approaches), the use of direct numerical simulation (DNS) as a methodology for advancing modeling capability, and the predictive capability and use of Reynolds-averaged Navier–Stokes (RANS) models. These topics were discussed in a broad context as well as in the context of "extreme" conditions.

Several possible high-impact research directions were discussed. In the absence of well-defined experiments and detailed data that can elucidate the "credibility gap", four priority research areas that could dramatically improve predictive capability in a transformative way were identified for theory and modeling (and are further discussed in section 3.3 below):

1. Further theoretical development of multiphysics and nonequilibrium model equations.
2. Development of modeling frameworks for the simulation of multiscale flows in extreme conditions.
3. The use of physics and evolution equation-based scaling analysis to specify the regions of parameter space and solution metrics relevant to extreme applications.
4. A proposal for a *Material Mixing Olympiad*.

The last of these can serve as cross-cutting modeling, simulation, and experimental objectives that gauge progress in the areas addressed in the workshop, as well as progress in integrating these areas towards the longer-term goal of predictive modeling of mixing in extreme environments. This section concludes with a 5, 10 and 15 year outlook intended to indicate future scope, and reflect simulation and experimental needs that are addressed below in sections 4 and 5.

3.2 Current Capabilities and Needs

3.2.1 Introduction

An important objective within the theory and modeling community is the development of reduced descriptions of turbulent mixing and processes coupled to the evolution of complex hydrodynamics flows: such descriptions must balance accuracy with cost effective simulations. This objective is both a driver for the priority research directions for simulations/predictions and for experiments/diagnostics discussed in sections 4 and 5, respectively, as well as the beneficiary of the data generated through execution of these directions. In general, the reduced models must account for the flow complexities summarized in section 3.1 and include a broad spectrum of initial conditions, range of scales, and extreme parameter regimes (e.g., Re ~ 0–10^{10}, At $\sim 10^{-3}$–1, Sc $\sim$ 10^{-4}–10^{3}, and Ma $\sim$ 0–100).

The three simulation and modeling approaches used are direct numerical simulation (DNS), various forms of large-eddy simulation (LES), and various forms of Reynolds-averaged Navier–Stokes (RANS) modeling. A proper DNS (see section 3.2.4) resolves all scales and material interfaces with no averaging, and yields full three-dimensional data for all fields that can be further analyzed to develop insight into complex flow physics. The various approaches to LES (see section 4.3.5 for a more detailed codification) resolve the "largest" scales and solve explicitly or implicitly "filtered" forms of the Navier–Stokes and constitutive relations with

subgrid-scale models used to represent unresolved correlations using resolved-scale fields. LES yields only resolved-scale fields, and the interpretation of what precisely these fields represent is not entirely unambiguous. The various hierarchical approaches to RANS models ensemble- or statistically-average the Navier–Stokes and constitutive relations with auxiliary modeled turbulent transport equations used to formulate closures for correlations using the mean fields. In recent years, DNS and LES have been increasingly used to aid in the assessment of RANS models, especially in the broader turbulence community. The relative advantages and disadvantages, as well as limitations, of these approaches are discussed below and further in section 4.

3.2.2 Predictive Modeling

The development of a robust predictive theory and modeling capability is essential for progress in material mixing in extreme environments, partly because of the inherent difficulties associated with the fidelity of experiments and diagnostics. When discussing modeling, "predictive capability" must be distinguished from "postdictive capability". Presently, most modeling is postdictive in that results from experiments that are the *targets of prediction* are known in advance. A salient point here is the assessment of the implications of code calibration (widely used in simulation of complex systems) on predictive capabilities. Calibration requires some information about the targets of the prediction, leaving a question about which other observables (not used directly for calibration) can be regarded to have been predicted. Further discussion of calibration is included below in sections 3.2.6 and 4.3.2 with a more detailed discussion of predictive modeling and simulation presented in sections 4.1 and 4.2. In general, the metrics of prediction must be clearly defined and may include, but not be limited to, some mean or variance or a quantity depending on an outlier, e.g., a set of failure metrics.

The modeling community should evolve towards the routine use of some appropriate form of uncertainty quantification (UQ) to accompany a set of predictions (e.g. Le Maître and Knio, 2010). Examples of such UQ could be as simple as error bars quantifying the uncertainty in a set of model predictions, or the application of a more elaborate UQ methodology to an ensemble of simulations on which the predictions are based (indeed, it is now common for archival journals to require uncertainty analysis). Concomitantly, an appropriate form of UQ should also accompany the experimental observables, which are the target of the predictions. It should be noted that the concept of a formalized and meaningful UQ methodology is not unanimously accepted. In justifying the quality of a set of predictions, emphasis should be placed on the fidelity of physics inputs and physics-based modeling that underpins that set of predictions. Generally accepted UQ methodology and practice are discussed further below in section 4.3.2. Two remarkable examples of predictions that predated and motivated experiments are the Taylor (1950) and Richtmyer (1960) predictions of Rayleigh–Taylor and Richtmyer–Meshkov instability.

3.2.3 Limitations or Failures of Classical Models

In assessing the current state-of-the-art in modeling complex hydrodynamics and turbulent mixing, it is helpful to review examples of classical theoretical and numerical modeling approaches that fail under known conditions. For the present discussion the "classical model" is defined as the multicomponent, compressible Navier–Stokes equations for Newtonian fluids

(Williams, 1985) to include appropriate equations of state and a self-consistent prescription of molecular transport coefficients (Cook, 2009).

There are several examples of classical model failures in the regime of gas dynamics. It is well-known that the above classical description fails to describe the dynamics when the mean-free-path becomes an important length scale, e.g., the internal structure of moderate-to-strong shocks (which may or may not be important for a given application) (Josyula et al., 2011). A second example is a converging shock at the time of shock impact on an origin or axis in which an Euler description predicts a singularity (e.g., axisymmetric flow) and the Navier–Stokes description breaks down as a result of mean-free-path (Tamm, 1965), dissociation (Boyd et al., 1995), ionization (Grasso and Capano, 1995), and other phenomena.

The classical description of reacting or combusting flows breaks down in regimes of both thermal and chemical nonequilibrium (Demirel, 2007). The widely used Fickian diffusion approximation (Fick, 1855; Bird et al., 2001) is also inapplicable in flow regimes characterized by extremely strong pressure, temperature, or concentration gradients. In such extreme regimes, it is necessary to generalize the mass molecular flux of a fluid to include a sum of diffusive fluxes corresponding to mass diffusion by concentration gradients, pressure gradients, external forces, and temperature gradients. The self-consistent determination of the transport coefficients may then require the solution of the Stefan–Maxwell equations (derived from the kinetic theory of dilute gases) determining the mass molecular fluxes (Curtiss and Hirschfelder, 1949; Curtiss and Bird, 1999). Such a procedure should also account for nondiffusive fluxes induced by locally nonequilibrium physical processes.

Other flows that cannot be described solely by the deterministic fluid dynamics equations are those that require some form of probabilistic or stochastic description (Risken, 1989; Gardiner, 1996) such as those exhibiting small-scale Brownian motion.

3.2.4 Direct Numerical Simulation and its Uses

With increasing computational capabilities and exascale computing on the horizon (see section 4.3.3), direct numerical simulation (DNS) (Moin, 1991; Härtel, 1996; Leonard, 1996) is becoming more widely used in fundamental studies of turbulence and turbulent mixing. DNS is based on equations that mathematically describe a hypothetical continuum, with no reference to a discretization. The procedure for solving the equations using DNS then requires an adequate numerical algorithm to obtain a (nearly) grid-independent solution with appropriately small numerical errors (Jiang and Lai, 2009). The convergence properties of the numerical solutions to the discretized equations are a separate issue. A specific set of DNS equations may not be adequate or applicable in particular physical regimes, which requires that an improved set of equations be developed theoretically.

As a numerical technique, DNS is a concept originating in incompressible, constant-density turbulence: its extension to more complex variable-density or compressible turbulent flows (Lele, 1994) including interfacial turbulent mixing must be carefully defined. This extension is particularly problematic when discontinuities exist in the flow (e.g., shocks, material interfaces, and distinct molecular transport coefficients for different species). There are many possible elements of a definition of DNS. First, the equation set to be solved numerically using DNS must

represent a closed, well-posed, initial-boundary value problem. Such a set should contain well-defined molecular transport coefficients, constitutive relations, and equations of state that are independent of the particular discretization scheme and numerical algorithm used to solve the equation set. For the results of a given DNS to be meaningful with respect to the fundamental study of turbulence and mixing, the equation set should allow for convergence tests with increasing spatial and temporal resolution that permit convergence rates to be obtained for a given numerical method. One panel member offered a much more restrictive definition of what DNS means practically: that the equation set *must* contain the details of the discretization, i.e., the fields obtained from DNS are always dependent in some fashion upon the details of the numerical solution (grid resolution, numerical algorithm, etc.). Limitations of DNS and areas for further development, particularly in the context of turbulent mixing, are discussed in section 4.3.6.

An important use of DNS, and in particular DNS with deliberately chosen modified equations or boundary conditions, is to elucidate the detailed flow physics responsible for some observed macroscale phenomena (Moin and Mahesh, 1998). With appropriate resolution as demanded by the Kolmogorov and Corrsin–Obukhov scales and a sufficiently large ensemble, DNS provides data on all structures and statistics in a given flow field. However, DNS of physically realistic and relevant turbulent flows is meaningful only in three dimensions, and despite advances in computation over the last decade, high-resolution DNS still engenders very high computational and data storage/processing requirements. Additionally, DNS requires high quality (generally, higher-order accurate spatial and temporal) algorithms. Many direct numerical simulations represent an idealization of a particular flow, due to the complexities in precisely specifying initial and boundary conditions and other relevant flow parameters. However, numerical experiments using DNS have begun to synergistically utilize advances in experimental diagnostics to provide detailed data needed for initial conditions representative of laboratory experiments (Mueschke and Schilling, 2009a) and yield data that has not yet been measured (Mueschke and Schilling, 2009b).

DNS is often applied to flows outside the paradigm of incompressible, constant-density turbulence. For the *bona fide* use of DNS as a surrogate for physical experiment (for example, when experimental data is either unavailable or very difficult to obtain), there should be a very high degree of confidence in the applicability of the equation set in the target regime—the *proper* DNS of a given equation set is a separate issue from the domain of correct physical applicability of the set. DNS extrapolated to other regimes should be used, and its predictions interpreted, with caution. Although extremely challenging, and generally unavailable even for the incompressible Navier–Stokes equation, it is desirable from a mathematical and physical perspective to eventually establish long- or finite-time existence proofs for solutions of the equations describing turbulence and mixing induced by hydrodynamic instabilities.

In recent years, DNS of compressible turbulence using kinetic theory-based methods has been successfully demonstrated. Two such approaches are the lattice Boltzmann method (Succi, 2001; Aidun and Clausen, 2010) and the gas-kinetic method (Xu et al., 2008), both of which have been applied to small Mach number flows and found to be reasonably accurate compared with spectral and finite-difference DNS of the Navier–Stokes equations. Thus, the proof of concept of Boltzmann equation-based DNS has been established. In principle, Boltzmann

equation-based methods do not require closed form constitutive relations or macroscopic transport coefficients. Therefore, these methods are promising for nonideal flows involving moderate nonequilibrium and noncontinuum effects, multicomponent/multiphase effects and stochastic reactions relevant to material mixing. However, major challenges remain in realizing the full potential of these methods including the proper DNS of:

1. Nonthermochemical equilibrium flows.
2. Multiscale and multiphysics flows.
3. Flows in the absence of closed constitutive relations.
4. Flows with finite-rate chemistry involving multicomponent or multiphase effects.

The systematic development of such kinetic theory-based methods can greatly benefit the study and possible control of mixing in extreme environments.

3.2.5 Large-Eddy Simulation and Subgrid-Scale Modeling

The high computational expense associated with DNS has been a major motivation for developing a reduced simulation paradigm based on resolving only the largest scales and modeling the effects of the unresolved (subgrid) scales on the large scales using subgrid-scale models—large-eddy simulation (LES) (Lesieur et al., 2005; Sagaut, 2006; Berselli et al., 2006). Limitations of various approaches to LES and areas for further development, particularly in the context of turbulent mixing, are discussed in section 4.3.5. Most formulations of the large-eddy equations rely either on explicit filtering (Aldama, 1990) or on implicit filtering provided by the numerical discretization (Grinstein et al., 2007). Added complications for explicit filtering are filtering near boundaries and commutation errors (Ghosal and Moin, 1995; Ghosal, 1999). Implicit filtering and subgrid-scale modeling provided by physics-capturing numerical algorithms is the basis for implicit LES (ILES), discussed in more detail in section 4.3.5 and elsewhere (Sagaut, 2006, Grinstein et al., 2007). More recent paradigms for LES involve neither explicit nor implicit filtering, but represent the unclosed Reynolds stresses and turbulent fluxes using turbulent viscosities and diffusivities. An example is the artificial fluid LES of compressible turbulence and mixing (Cook and Cabot, 2005; Cook, 2007). An important conceptual advantage of this approach is that there is no filter scale; however, it is then unclear which scales are resolved and which are subgrid. Yet another approach to LES is explicit structure-based modeling such as the stretched-vortex subgrid-scale model (Hill, Pantano and Pullin, 2006; Chung and Pullin, 2009), in which the filtering paradigm is used as a guide to modeling (but is not followed rigorously) with emphasis on physical modeling of subgrid dynamics.

As in the case of DNS, large-eddy simulation is only meaningful in three dimensions and similarly requires high quality algorithms. Additional complications arise when arbitrary, unstructured grids are used and when discontinuities are present: algorithms designed for DNS or LES of incompressible flows may not be suitable and may not be sufficiently robust. While numerical algorithms based on (higher-order formally accurate) shock-capturing techniques are attractive, they introduce numerical errors that can contaminate the flow field, especially in smoother flow regions away from the discontinuities. A well-known example of where the underlying numerical algorithm in an LES can have a significant effect on the representation of the subgrid physics is the study of the relative importance of aliasing and truncation errors compared to the magnitude of the subgrid-scale model terms, where it was shown that

truncation errors can exceed the magnitude of the subgrid-scale terms in low-order finite-difference LES (Ghosal, 1996, 1999; Geurts, 2006). In general, and unless shown otherwise, the results of an LES or ILES depend on grid resolution (Vreman et al., 1996; Meyers et al., 2003; also see Bose et al., 2010) and on details of the explicit or implicit subgrid-scale models. See Chung and Pullin (2010) for an attempt to address this issue by subgrid-continuation for some turbulence quantities. Like direct numerical simulation, LES is largely a concept originating in incompressible, constant-density turbulence, and its extension to complex and compressible flows must be systematized. For the reasons enumerated in section 3.1, the theoretical formulation of the large-eddy equations and the related interpretation of the equations for turbulent flows with material mixing are nontrivial for complex multiphysics flows, and presents both challenges and opportunities as discussed further in sections 4.3.1 and 4.3.5.

For free turbulent flows, the applicability and success of subgrid-scale modeling is largely predicated on the universality and scale-invariance properties of the small scales in "canonical" turbulence at large Reynolds numbers (Meneveau et al., 1999a,b; Meneveau and Katz, 2000). Practically, this means that an LES must have sufficiently high resolution to encompass some (perhaps very short) range of scales in an inertial subrange characterized by relatively simple scaling laws. Provided that this is the case, the success of many subgrid-scale modeling approaches relies on providing a largely dissipative process in which energy is cascaded from the resolved scales through some inertial subrange and then dissipated at the subgrid scales by the model. However, for the "extreme" turbulent flows considered here that are characterized by one or more of the properties enumerated in section 3.1 (e.g., anisotropy, inhomogeneity, presence of discontinuities, baroclinicity, varying density, strong compressibility, nonequilibrium, transitional and unsteady flow) the requisite conditions needed are clearly not satisfied. Consequently, most of the available models do not have any theoretical basis for being potentially successful. An example is Rayleigh–Taylor turbulent mixing in which the flow is not driven by the large scales, but rather grows from very small (perhaps subgrid) scales until large-scale structures eventually appear. In this case, the required resolution of the LES is virtually that of a DNS (Cook et al., 2004). Given the range of parameter values likely in extreme turbulent material mixing (briefly summarized in section 3.2.1), it is unclear whether adequate computing power will be available for LES using subgrid-scale models based on the "canonical" assumptions.

Various approaches to subgrid-scale modeling have relative advantages and disadvantages, particularly for specific flow categories. Perhaps a testimonial to the fact that there is no consensus on what the best models are is the large variety of available models: eddy (hyper)viscosity/diffusivity and backscatter models; one-equation models; scale-similarity, gradient, and mixed models; structure-based models; fractal and multifractal models; deconvolution models; wavelet models; variational multiscale models; and, dynamic versions of many of these models. Rigorous results for the analysis of subgrid-scale models and LES are very limited, but some are available in the context of finite-element analysis of incompressible flows (John, 2004; Berselli et al., 2006).

3.2.6 Predictive Capability and Uses of Reynolds-Averaged Navier–Stokes (RANS) Models

While DNS and LES continue to have an expanding role in the study of turbulent mixing, they remain too computationally expensive and otherwise conceptually limited to be routinely used for applications. For example, the design cycle for new inertial confinement fusion (ICF) targets requires a very large number of simulations to explore a given parameter space (Lindl, 1998; Atzeni and Meyer-ter-Vehn, 2004). Changes in material composition, dimensions, shock timing, estimates of capsule surface roughness, and many other parameters typically require a new simulation for each change to quantify the performance of the target for given laser driving conditions—this can easily lead to hundreds or even thousands of simulations before a final design conclusion can be reached. For this reason and for conceptual and computational limitations (Lumley, 1978; Pope, 2004) of DNS and LES for complex mixing hydrodynamics, it is essential to develop and utilize alternative reduced descriptions of the key turbulent and mixing processes.

The most common modeling paradigm used for ICF design (Takabe, 2004) is Reynolds-averaged Navier–Stokes (RANS) modeling (Pope, 2000; Durbin and Pettersson Reif, 2001; Chassaing et al., 2002). Such statistically-averaged descriptions have diverse formulations, including two-equation, algebraic stress, gradient-transport, and second-order closure models, each having their unique strengths and weaknesses. Depending on the level of detail required for a given set of predictions, RANS methods have relative disadvantages compared to DNS and LES (Pope, 2000, 2011). Nonetheless, the engineering RANS approach for predicting the statistics of a large class of turbulent flows may be useful, or indeed all that is needed, for a particular set of target predictions. For example, when the symmetries of a given flow can be used to reduce the problem to a statistically one- or two-dimensional description, RANS models have a significant computational advantage over DNS and LES, especially for flows having a large parameter space. RANS models do not resolve any length scales in a turbulent flow.

From a theoretical perspective, the classes of turbulent flows for which a RANS description is likely to be useful are those in which:

1. Multipoint correlations are self-similar and can be characterized by a one-point statistical description.
2. The flow is expected to reach a self-similar state (Sedov, 1993; Barenblatt, 1996).
3. A single time and length scale is dominant.

Advanced second-order moment equations (Speziale, 1991, 1996, 1999; Hanjalić and Jakirlić, 2002) and more rigorous turbulent dissipation or length scale equations require less reliance on gradient-transport hypotheses, and the last two requirements become less important.

The typical paradigm for engineering use of RANS models is (Dimonte and Tipton, 2006; Chiravalle, 2006; Banerjee et al., 2010):

1. Develop a model that satisfies several different physical and mathematical limits, and is consistent with experiments.
2. Calibrate against available experimental and/or simulation data.
3. Test by postdiction against other data.
4. Use for prediction in other regimes where data is unavailable.

In the material mixing field, two items in the model development process have not been fully utilized to date: (1) the development of closure models based to any degree on a mathematical theory (e.g., tensor basis expansions, realizability, asymptotic analysis) and; (2) the predictive application of such models with adequate experimental and simulation data (with specified uncertainties) over a wide parameter space for a priori and a posteriori model assessment. Thus, RANS models should be used cautiously for prediction, with the range of applicability of a given model determined if at all possible.

3.3 Priority Research Directions

3.3.1 Advanced Multiscale, Multiphysics Models

Most models presently developed for mixing processes have been primarily directed at describing growth of mixing layers in simply forced flows. However, both the requirements in applications and the available computing capacity for simulation, modeling, and model validation mean that it is an urgent priority to advance from predicting mixing layer growth towards the prediction of statistics. There is a clear need for further development of multiscale, multiphysics theoretical and numerical models including the following highly desirable properties. First, the models should be based strongly on the underlying physics of the flow and have a firm analytical/mathematical foundation. Second, they must account for interactions between the flow and equilibrium and finite-rate chemistry, transport processes, material strength, change of phase, and complex external interactions.

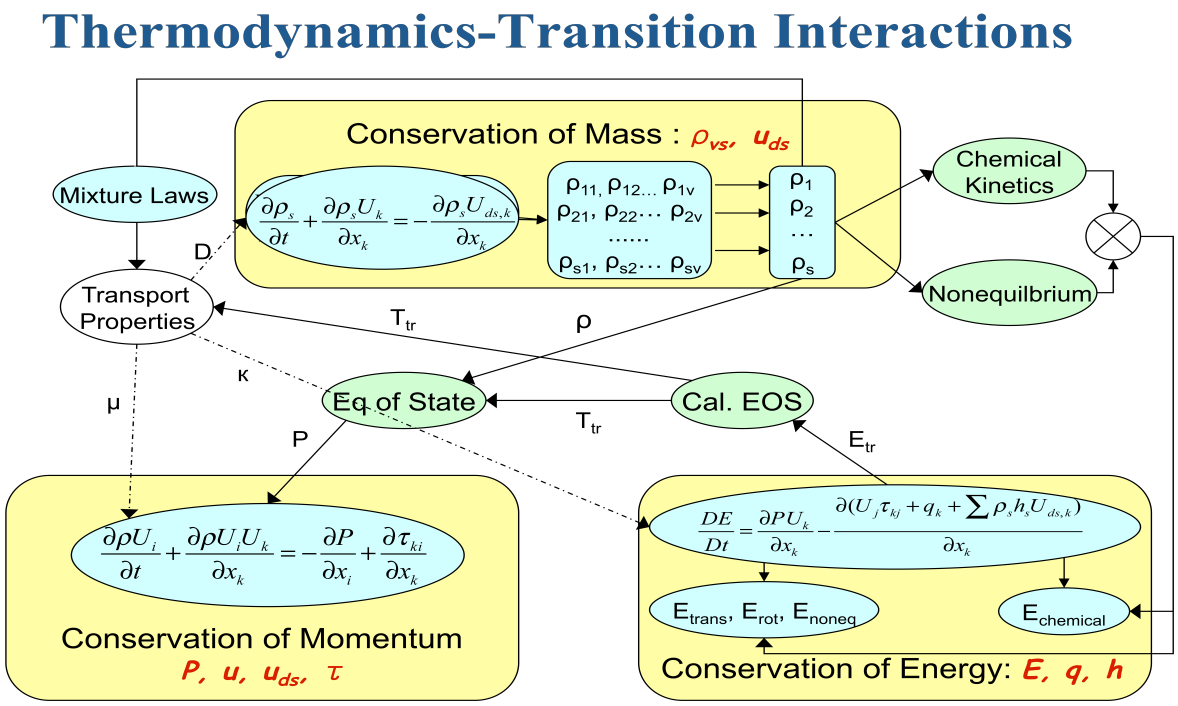
Methodologies to be developed and applied could include but are not limited to nonlinear enslavement (Dubois et al., 1999; Berselli et al., 2006), structure-based methods for the coupling between the meso- and macroscales (Lesieur and Métais, 1996; Misra and Pullin, 1997; Pullin, 2000), and other subgrid-scale models (Lesieur et al., 2005; Sagaut, 2006). The further development and validation of more advanced subgrid models that could form the basis for both implicit and explicit unresolved hydrodynamics (e.g., for RANS, LES, and hybrids of these) is required to develop longer-term predictive modeling and simulation capability: the development of these mesoscale simulations will drive and test models and codes at the extremes of present capability, which may then be applied directly in experimental assessment when suitable facilities become available (see section 5 for examples). The development of these models will rely on a hierarchy of validation, ranging from experiment and DNS at the finest scales, through LES at coarser scales, to RANS models typically used for engineering applications. Model development should not be limited to analytical formulation and a posteriori assessment, but should also incorporate a framework for rational comparison to simulations, experiments, and theory (see Oberkampf and Barone, 2006; and section 3.3.4).

3.3.2 Frameworks for Nonequilibrium Flows

In addition to the development of advanced multiscale, multiphysics models with the properties described in section 3.3.1, there is a need for models and theoretical frameworks suitable for describing both thermally- and chemically-nonequilibrium flows (Stalker, 1989; Köhler and Wiegand, 2002). Such models should include a number of characteristics: (1) they should contain finite-rate reactions that occur, for example, in ICF applications and supernovae, and; (2) they should incorporate thermodynamic equation-of-state-type closures that extend

beyond equilibrium conditions (Ortiz de Zarate and Sengers, 2006). It should be possible to extend the modeling framework to macroscopic (e.g., Burnett) or kinetic (e.g., Boltzmann) descriptions. Examples of flows for which such capability is needed include combustion or large Schmidt number nonequilibrium flows (see section 5 for possible experiments). In high-energy-density physics regimes, plasma effects (which may include electromagnetic interactions) should also be included (Drake, 2006).

Interaction Framework. To establish the precise nature of the influence of nonequilibrium thermochemistry on velocity fluctuations, the interplay between mass conservation, momentum balance, energy balance, species balance, and equations of state must be established. The anticipated outcome is a framework for thermochemistry–transition interaction with clear identification, characterization, and parameterization of the manner in which surface chemistry, gas chemistry, and nuclear/quantum chemistry individually and collectively affect the evolution of velocity fluctuations. Figure 1 schematically shows the interactions between the various conservation/balance and state equations. The species balance equation contains the chemical nuclear/quantum reactions represented by appropriate kinetic mechanisms. Heat release physics is described by the energy equation.



Nonequilibrium thermochemistry effects are manifested on Navier–Stokes velocity fluctuations via the: (1) density field; (2) pressure field and; (3) transport properties. This indicates that the thermochemistry and fluid computations can be modular. The thermochemistry module must provide the density, pressure, and transport coefficients, which will be used in the flow computational modules to assess their influence on the velocity field.

Thermochemistry module. Thermochemical processes occur on time scales vastly different from those of the flow processes. Air chemistry and nuclear/quantum chemistry can also occur on different time scales, further exacerbating the computational challenges. This makes reacting/relaxing flow simulations even more computationally intensive than traditional transition simulations. For the foreseeable future, it will not be possible to couple a high-fidelity flow solver with detailed thermochemistry, as each can be extremely computationally demanding. Experiments that can address improving the understanding of complex thermochemistry are needed.

Thermochemistry–fluid dynamics interface module. The purpose of the interface module is to generate hydrodynamic pressure from the translational energy using appropriate calorific and state equations. The assumptions here should be consistent with those in the thermochemistry module. This module will also generate the transport properties using applicable mixture laws. The outputs from the interface module are all of the thermodynamic and transport properties needed to solve the Navier–Stokes equations.

3.3.3 Application of Scaling Concepts

Material mixing at extremes is usually associated with conditions dramatically departing from those under which canonical turbulence is expected to occur. Compared to isotropic, homogeneous, and statistically-steady turbulence, these departures may include different scalings, spectra, structure functions, correlations, and interscale couplings. “Extreme turbulence” may also include qualitative distinctions, such as coherence and randomness of statistically-unsteady mixing flows, and sensitivity to initial conditions. Some additional perspective on these issues is offered elsewhere (Abarzhi and Sreenivasan, 2010; Abarzhi, 2010). A stronger emphasis on the application of scaling concepts and related theoretical analysis to the flows relevant to material mixing in extreme conditions (Ryutov et al., 1999) is thus essential for providing guidance to the development and application of modeling, simulation, and experiments. Dimensional analysis and the identification of dominant dimensionless groups in complex compressible high-energy-density turbulent flows will be invaluable for better understanding the range of physical conditions for which theory, equations, and reduced order models need to be developed. The analysis should also provide the experimental and simulation communities with specific quantities to be measured for better understanding unresolved dynamics needed in reduced order (e.g., LES and RANS) models, as well as aid in designing these experiments.

3.3.4 A “Material Mixing Olympiad”

The preceding three priority research directions suggest a fourth in the form of a “Material Mixing Olympiad,” similar to the previously held Stanford University “Turbulence Olympiads”. A proposal is to hold two Olympiads; the first in five years based on extensions of present day experimental diagnostic capabilities, and a second in fifteen years based on new and as yet unknown advances in the fielding and diagnosis of experiments. Such Olympiads could include the following. It is desirable to identify and carefully define two or more “canonical” experiments, each performed by two different experimental groups and preferably on different facilities. The experiments would use well-resolved diagnostics that would reach to smaller scales than presently attainable using existing diagnostics. The experiments should be designed

a priori so that they could be used to discriminate between various models for unresolved hydrodynamics and different theoretical approaches. The accuracy, resolution, and dynamic range in the experiments should be chosen such that their results can be compared as closely as possible to model predictions. The experiments should include an accurate quantification of systematic experimental errors and their influence on the measured quantities. A set of well-defined detailed diagnostics would be specified as targets for model prediction. The theoretical, modeling, and simulation predictions would be tested against the experimental data without prior knowledge of that data. Some relevant regimes could include large Reynolds number, large Schmidt number, and large Mach number flows. One experiment could be performed at high energy density and may involve non-Newtonian materials. Section 5 presents ten possible candidates for the Olympiad, with more details given in the Appendices.

3.4 Cross-Cutting Issues

3.4.1 Opportunities

As progress continues to be made on the priority research directions identified above, it is essential to continually assess the progress in achieving the objectives summarized in these research areas. For this purpose it may be helpful to apply two criteria: *what is the current state of predictive capability* and *how predictive do these capabilities need to be*? The role of the first criterion is clear. The second criterion pertains to the level of reliability and accuracy required of various predictions, which is determined by the confidence that is needed in them. This, in turn, is related to the use that will be made of the predictions. These two criteria are (or can) also be directly addressed by Predictions/Simulations and Experiments/Diagnostics: thus, they form a cross-cut to other activities and problems discussed below.

Several specific cross-cutting issues with Predictions/Simulations and Experiments/Diagnostics can be identified. The application of VVUQ principles traditionally used for simulations should become standard practice for developing a rational basis for systematic and rigorous assessment of turbulence model predictions. This, in turn, could potentially provide useful guidance for quantifying how accurate DNS and LES must be for specific model development and validation studies. The successful exploitation of exascale computing applied to grand challenge flows with turbulent mixing will have several benefits. The elucidation of the mixing transition in different classes of flows (see section 4.3.7) can strongly influence the further development and validation of reduced model descriptions. In addition, exascale-class computing can potentially allow an ensemble of simulations to be performed tractably in order to extract true statistics for comparisons to model predictions. Research in the proper formulation of DNS and LES for material mixing in extreme conditions, which includes the interplay between the physics represented by the continuum equations and the discretization can have a positive impact on: (1) development of higher fidelity datasets for model analysis and (2) better understanding and mitigating the inevitable interaction between physics and numerical algorithms in RANS models for turbulent mixtures and interfacial flows.

In the Experiments/Diagnostics area, perhaps the most important cross-cutting issue is the close coordination between the modeling and experimental community in the design of future well-diagnosed experiments. Higher fidelity experimental data (for example, as detailed in Appendix C) acquired over a wider parameter range than presently accessible and with

quantified errors can have a dramatic impact on the development of more advanced and more predictive reduced models. For example, it would be highly desirable to extend the successes of the comparisons between conditionally-averaged experimental data and LES both a priori and a posteriori (Meneveau and Katz, 1999; Liu et al., 1999; Tao et al., 2000; Chen et al., 2005; Chen et al., 2006; Kang and Meneveau, 2008) to interfacial mixing flows.

3.4.2 Goals for Short-, Intermediate-, and Long-Term Progress

As part of the identification of high-priority, high-impact research directions, goals for predictive turbulence, mixing, and materials modeling capability were established for short-term (1–5 years), intermediate-term (5–10 years), and long-term (10–15 years) progress.

1–5 year timeframe. It is desirable to model a wide class of multicomponent, compressible turbulent flows in planar and converging geometries. These include acceleration-, shock-, and shear-driven turbulent processes and mixing induced by Rayleigh–Taylor, Richtmyer–Meshkov, and Kelvin–Helmholtz instabilities, and homogeneous variable-density turbulence. Shock stability in convergent geometries is likely to be an important issue that may require full cylindrical or spherical geometry in numerical simulations. In addition, flows subject to strain, compressive–expansive turbulence (Coleman and Mansour, 1991, 1993; Zeman and Coleman, 1992; Blaisdell et al., 1996), and shock–turbulence interaction (Hussaini et al., 1986; Andreopoulos et al., 2000) can provide additional stringent tests of models. To begin considering modeling of mixing in extreme conditions, it is desirable to add flows driven and affected by volumetric deposition of energy. The effects of complex bounding geometries may also be relevant.

5–10 year timeframe. It is desirable to first model coupled/combined instabilities, as these are typically what occur in ICF and supernovae (rather than isolated instabilities). Additional couplings can then include:

1. Radiation- and MHD-driven plasma flows.
2. Chemical and thermonuclear reactions.
3. Impact-driven flows with phase changes including strength, damage, and spall.

10–15 year timeframe. A “grand challenge” would be to further include noncontinuum, nonequilibrium, and other nonideal processes. The multiscale, multiphysics modeling would necessarily include scales introduced by noncontinuum (e.g., kinetic) descriptions.

4. Predictions and Simulations (F. Grinstein and W. Rider)

4.1 Summary

During the workshop we discussed the key challenges associated with simulating material mixing fluid dynamics. We started by describing "Predictive Simulation" and during the course of the workshop identified four key research priorities: interface dynamics, VVUQ (verification, validation and uncertainty quantification), exascale computing, and systematic model development and assessment for the physics of turbulent mixing. The next paragraphs introduce our interpretation of predictive simulation, and the four key research priorities. The sections thereafter provide a detailed description, and we close this chapter with a discussion of cross-cutting issues.

In section 4.2 we address the concept of predictive simulation with an established verification and validation pedigree. Domains of applicability for the simulation models and their calibration used in the simulation must be established by well-defined procedures. Being predictive involves establishing verification and validation (VV) procedures to evaluate the quality of the simulated solutions, and well-defined metrics for uncertainty quantification (UQ). In particular, being predictive is the ability to predict a result without pre-existing experimental (or DNS as applicable and available) knowledge for that specific case with quantified uncertainty/confidence and established VVUQ. An important focus is on establishing the quality of reference data (DNS, laboratory experiments or observations) for intended purpose and suitability for validation.

Section 4.3 describes the priority research directions and starts in 4.3.1 with the accurate and reliable simulation of the dynamics of material interfaces as essential for material mixing fluid dynamics, and may be the largest single source of systematic error. There exist a number of outstanding challenges in the area arising from the relative weakness of theoretical foundations associated with the models and techniques available for simulation. Without a solid theory when solving complex problems, the solutions are potentially without definable quality control.

The discussion in section 4.3.2 addresses VVUQ as being essential to quality control and proper communication of simulated results. VVUQ is complex and hierarchical in nature. The characteristics of VVUQ elements depend upon where the VVUQ activity takes place in the hierarchy of physics and models. The process discussed here has been addressed by many researchers (AIAA, 1998; ASME, 2006; Oberkampf and Roy, 2010). Despite all that has been written about VVUQ, there remain diverse and often imperfect definitions for each element of the process. Nonetheless, VVUQ is essential for simulating dynamic material mixing.

Section 4.3.3 continues with exascale computing that offers the promise of a thousand-fold increase in supercomputing power in the next decade. The challenges associated with achieving this power are profound (Keyes, 2011). Nonetheless, exascale computing can address a host of science and national security applications. Key architectural challenges remain unsolved with many parallel paths being followed on power, memory, interconnection networks, and resilience. Exascale computing offers difficult challenges for numerical methods, but also the

promise of transformative computational capability. For example, in the next decade to 15 years we should be able to compute the "mixing transition" (Dimotakis, 2000) through direct numerical simulation.

Sections 4.3.4 to 4.3.6 identify the need for systematic model development and assessment as a priority research direction. In particular, the process for developing and assessing RANS turbulence models and LES is often *ad hoc* and lacks a systematic approach. For progress, this must change to include the VVUQ methodology in the development and assessment process. Furthermore, turbulence models coexist with numerical integration schemes, but often are not coordinated. It is well known that numerical errors can be extremely harmful to many LES methods (Ghosal, 1996), and perhaps this provides a motivation for reliable DNS (Moin and Mahesh, 1998). For implicit LES (Grinstein et al., 2007) the numerical method is the "model", and the needs of the physical circumstance should play an intimate role in the design of the numerical method. Where RANS modeling is used, the material interface tracking methodology can greatly impact the results. The greater awareness of the modeling issues by the numerical methods would offer a significant advance. Section 4.3.7 identifies a priority grand challenge, namely, "Material Mixing Transition".

The section closes in section 4.4 by identifying cross-cutting issues.

4.2 Definition of Predictive Simulation

Predictivity in numerical simulation is the ability to produce a result without pre-existing experimental knowledge for that specific case, with quantified uncertainty (and/or confidence) and an established verification and validation pedigree. The ability to predict a result should not rely upon case-specific calibration although many models will be calibrated as part of a disciplined approach to hierarchical validation. The model should be verified and documented including a detailed and professional software development effort to implement the model and its numerical solution. Uncertainty quantification could be accomplished using intrusive and/or nonintrusive methods, and should include estimates of numerical error associated with the discretization of the model. The model itself should be validated against related experimental cases to provide confidence in its applicability.

The key question is "What are you trying to predict?". To make the prediction process well-defined it is essential for metrics that are predicted to be well-defined. This definition should include both the computational and experimental instantiation of the measure. All metrics should in principle be accessible as experimental measurements, though practical constraints (e.g., cost, limits of available instrument technology) may make such measurements impractical. Often an application-specific metric is used because of its importance to the ultimate purpose for the predicted circumstance.

What activities are necessary to enable predictive simulation?

1. Experiments with UQ to be used for validation.
2. Solution verification (predicated on rigorous mathematics).
3. Code verification through a rigorous development and testing environment.
4. A rigorous UQ approach for addressing both aletory and epistemic uncertainties.

5. Disciplined calibration applied toward well-defined physical models (e.g., constitutive relations for materials).
6. Sensitivity analysis (aspiring toward as little calibration as possible).

Extrapolation is unavoidable when applying simulation to applications. This implies modeling for situations that are not captured with existing experimental data or observations. An archetypical example of the need for extrapolation is climate modeling, where the state being the object of simulation (climate in the future) cannot be known, and almost certainly not associated in full by any observations or experiments.

Finally, it is important that well-established domains of applicability for the models and their calibration used in the simulation be documented. These domains of applicability are important by-products of the VVUQ process (this topic is discussed earlier in section 3.2.2).

4.3 Priority Research Directions

4.3.1 Interface Dynamics for Predictive Material Mixing Simulations

The accurate and reliable simulation of the dynamics of material interfaces is an essential aspect in computing fluid mixing. Interfaces are intrinsic to the physics of mixing, and can have varying properties. Interfaces can be miscible or immiscible, with the character changing during the evolution of a system. This causes the numerical approximation to the physics to be extremely challenging because the basic features of the approximation should adapt to the evolution of the materials. For example, an interface may begin sharp and immiscible, but evolve into a state where it mixes at an atomic level with neighboring material (as it becomes a plasma, for instance). The numerical approximation with the greatest fidelity during the early time of a simulation becomes increasingly physically inappropriate when the interface changes its character in this manner.

Among the most pernicious issues associated with interfaces is the extreme sensitivity of most problems to the initial conditions. Indeed, relatively small variations in the initial state of the interface can result in large changes to the integral character of a mixing layer (Dimonte, 1999, 2000). This impacts the nature of the expectations from a simulation, almost necessitating a statistical viewpoint in comparing experiment with simulations. There exist a number of outstanding challenges in the area arising from the relative weakness of mathematical foundations associated with the techniques available for solutions. Where interface physics are concerned, the theory is largely missing. This is contrasted by shock wave theory, where convergence guarantees are based upon conservation and physically motivated entropy production (Lax and Wendroff, 1960; Leveque, 1990). These theoretical foundations have allowed shock-capturing methods to achieve great success in simulating a host of physical systems. For numerical approximations at material interfaces, such rigor is lacking.

Interfaces in general and, especially those in multiple dimensions, lack such a strong theoretical basis for their approximation. Better theory would enable the simulations to advance greatly with some degree of surety in results. Numerical methods for interfaces are based on much looser considerations than those for shock waves. For example, methods often involve no guarantee of conservation properties. Level set methods (Sethian, 1996) are archetypical in this regard. On the other hand, some entropy condition is available for the solution with level

sets based fundamentally on methodology borrowed from shock-capturing methods. Volume-of-fluid methods (Rider and Kothe, 1998) are conservative, but an entropy condition is not sensibly expressed by the method. It may have a capillary regularization associated with it, but there is little evidence that this rigorously provides a basis for confidence in the numerical results.

Several other methods are used extensively to simulate interface dynamics: interface tracking (Glimm, 1991) and high-resolution shock-capturing methods (Harten, 1978, 1983; Harten et al., 1987). Both methods have distinct advantages. The interface tracking method developed from shock tracking where the Rankine–Hugoniot relations are solved locally to move nodes in a moving boundary that describes the discontinuous flow. This methodology is typically nonconservative, but provides high accuracy through two mechanisms: the motion of the nodes through solving the exact mathematical relations for the interface/shock, and the differencing of the continuum equations on either side of the discontinuous surface. As the equations are not approximated across the discontinuity, the discontinuity does not pollute the accuracy of these solutions. The second approach involves the use of a shock-capturing method to approximate the material interface. Often this involves special techniques that remove as much numerical dissipation as possible (e.g., artificial compression). These methods have the advantage of conservation form and the satisfaction of entropy conditions. The solutions are not completely sharp and the material interface is slightly diffuse.

No single method is optimal for all circumstances. Perhaps the best option moving forward would be the development of adaptive-hybrid methods that provide the most physically appropriate approximation for the stage of evolution of the mixing. For example, a sharp interface method is optimal for many early stages of mixing, but as the flow evolves the mixing at small scales or the physical state of the materials dictates that the sharp interface approximation is inappropriate and potentially harmful to the fidelity of the solution.

A key question is “What type of conditions are needed to design an accurate, convergent, and reliable method?” For nonlinear waves such as shocks, the theoretical guidance given by the Lax–Wendroff theorem for captured shock waves is clear (conservation leads to weak solutions, entropy leads to uniqueness). Without this theoretical foundation for solving complex problems, the solutions are potentially without essential quality control and a basis for confidence.

4.3.2 Verification, Validation, and Uncertainty Quantification (VVUQ)

VVUQ underpins credible simulations. The results of numerical simulations are rarely precise and contain intrinsic uncertainty, quantitative estimates of which are needed to assess simulation quality. VVUQ plays a particularly acute role in computation supporting material mixing at extremes, forming a linchpin in the enterprise of predictive science, as described in section 4.2 (also see section 3.2.2). In coming years, the relevance of VVUQ to simulations of material mixing will increase and significant opportunities will arise. This role will only be amplified by the dual challenges of the physics-rich extreme regimes of interest and emerging exascale computing.

Verification of simulation software quantifies numerical errors and defines a rigorous basis for

believing that evaluation (AIAA, 1998; ASME, 2006; Kamm et al., 2008; Knupp and Salari, 2003; Oberkampf and Trucano, 2002, 2007; Oberkampf and Roy, 2010; Roache, 1998; Roy, 2005; Roy and Oberkampf, 2011; Stern et al., 2001; Trucano et al., 2003). Providing error estimates for complex problems falls under the purview of *solution verification* (also known as *calculation verification*, important for DNS as discussed in section 4.3.6), which generates quantitative assessments based on mesh sensitivity studies. The rigorous basis for solution verification estimates is achieved with *code verification*, which uses exact solutions to ideal problems. Together, these can be used to provide quantitative estimates of, e.g., discretization and iteration errors in solutions. These studies are distinct from *software verification*, i.e., checking for correct functioning of simulation software on a given platform using techniques such as unit and regression testing. Computational approaches for all verification activities are reasonably well established, although implementing them in simulation codes on emerging platforms will be an ongoing need.

Validation seeks to quantify the ability of a computational model to simulate a given application through comparison of computed results with a set of experimental data. Here, the model encompasses the governing equations, initial conditions, boundary conditions, constitutive relations, etc., instantiated through algorithms. Validation is discussed in many of the references cited above, as well as, e.g., by Hanson and Hemez (2001), Oberkampf (2001), Oberkampf et al. (2004), Sornette et al. (2007), and Stern et al. (2006). How to conduct validation poses many open issues, and application of validation techniques to material mixing simulations on exascale platforms will pose unforeseen challenges. Intimately related to validation is *calibration*, the process of improving the agreement of code calculations relative to a set of experimental data by adjusting code parameters. Calibration described, e.g., by Trucano et al. (2006), Kennedy and O'Hagan (2001), and Higdon et al. (2004), differs from validation in an important way in the manner by which experimental data sets are evaluated; moreover, the success of validation and calibration depends on verification results. Also related to validation is *sensitivity analysis* (SA), which comprises a set of evolving techniques to evaluate the variability (local and global) of computed results to input quantities, including parameters and models. SA can be used to help substantiate that a model is appropriate for the complex phenomena of interest (i.e., includes the essential sources of variability); this justification contributes to assessments culminating in the definition of validation and UQ tests. See the monographs by Saltelli et al. (2000) and Saltelli et al. (2004) and the work of Oakley and O'Hagan (2004) for discussions of SA techniques. The well-known Phenomenology Identification and Ranking Table (PIRT) approach (Trucano et al., 2002) can also be employed to define key requirements of planned validation analyses.

Uncertainty Quantification (UQ) comprises a host of rapidly evolving techniques by which to quantitatively estimate errors associated with a model, including experimental data and their uncertainties. These uncertainties have two general forms. *Aleatory* (*irreducible*) *uncertainty* describes inherent variation in a quantity of interest, while *epistemic* (*reducible*, *structural*, or *subjective*) *uncertainty* reflects lack of knowledge about this quantity. While probability and statistics can be used to evaluate aleatory uncertainty, the quantification of epistemic uncertainty (see Jakeman et al., 2010) is more difficult and will offer profound challenges to simulation of material mixing. An important part of UQ for numerical simulations is associated

with the discretization error inherent in calculations; see, e.g., Eça and Hoeckstra (2006), Roache (2009), Roy (2010), and Xing and Stern (2010) for discussions of numerical uncertainty estimation. More exotic approaches for UQ, including quantification of margins and uncertainties (QMU) (Helton, 2009), possibility theory (Dubois and Prade, 1998), and info-gap theory (Ben-Haim, 2006) may be useful in high-uncertainty circumstances of interest.

Verification, validation, calibration, SA, and UQ require substantial computing resources. One promise of exascale computing would be to in-line some of these approaches, say, by spawning multiple simulations for SA or UQ and their concurrent analysis. The software challenges of these will be great, as alluded to in section 4.3.3 below. A potentially valuable research avenue is the development of combined UQ/visualization capabilities on emerging platforms, to exploit increased processing power on material mixing simulation datasets.

The accuracy of the numerical solutions to multiphysics problems of interest is related to the fidelity of the solutions for simpler "component" problems, e.g., with fewer physical phenomena, simpler submodels, or reduced geometric complexity. Errors increase as one climbs the notional pyramid of problem complexity. This hierarchy is a useful paradigm by which to identify, e.g., where knowledge is insufficient, where empiricism is a placeholder for missing knowledge, or where additional calibration may be useful. This characterization can guide the development of *validation experiments*, which are designed to provide well-characterized data with quantified uncertainties for relatively simple problems (i.e., toward the bottom of the validation hierarchy) that are well-aligned with computational capabilities.

4.3.3 Exascale Computing

Although it is difficult to predict exactly what exascale computing will look like, it will require better memory management and a hierarchical computing structure, and the stability will likely be weaker. Memory management has, for nearly a decade, limited most simulations, and issues with memory management will be exacerbated with the heterogeneous architectures. It is likely that the highest capacity compute engines will become increasingly specialized, requiring code targeted to the architecture. Until the standardization of a software base is converged upon, code development on these architectures will be labor intensive.

The challenge of exascale is to determine the correct set of computational infrastructure and numerical algorithms to exploit these facilities. There may be cross-currents that are difficult to reconcile: whether it is better to group data by location within the mesh, or by physical type, may depend both on the algorithm to be used and the availability of vector-style facilities such as GPGPUs or on-chip vector accelerators. Changing to a higher-abstraction style of programming may help or hinder: for example, it is possible to write a simple DNS code in about 100 lines of Python that could utilize a GPGPU facility without source changes, but which sacrifices some part of its performance on any specific platform.

Although the extension of resolution (likely to be much less than an order of magnitude) is not dramatic for mixing studies, exascale offers several distinct advantages for turbulence studies.

1. Uncertainty Quantification: exascale machines can be used as capacity computing, allowing a thousand different instantiations of a particular problem currently solved on a petascale machine. Such calculations would be invaluable for uncertainty

quantification. We have identified UQ as a major issue in the future of turbulent mixing studies and this capacity computing use of exascale will be extremely valuable (see section 4.3.2).

2. In-line physics: the hierarchical computing structures in exascale will make it difficult to optimize codes with considerable communication. But local physics that can be calculated in line, such as detailed equation of state or opacity physics packages, will port more easily onto exascale architectures. Exascale will open up mixing problems requiring more detailed in-line physics (enabling techniques discussed in section 3.3).
3. Multiscale simulations: coupling higher order moment formulations (e.g., Grad's or Burnett equations) or atomistic descriptions (e.g., DSMC or even MD) to the Navier–Stokes equations to calculate on-the-fly material properties (viscosity, mass diffusion, temperature conduction, etc.) or describe small-scale effects where the continuum approximation fails (e.g., strong shocks, material discontinuities such as interfaces between immiscible materials or cracks) might be possible with exascale computing (enabling techniques discussed in section 3.3).

4.3.4 Systematic Reynolds Averaged Navier–Stokes (RANS) Model Development and Assessment

RANS modeling for extreme conditions and even the more benign conditions of everyday life continues to be driven by practical and theoretical concerns. The use of direct or large-eddy simulations (to be discussed in the following sections) are still and in the foreseeable future too expensive to overtake modeling efforts. Theoretically, one often needs not the instantaneous velocity, pressure, etc., fields, but the averages; and when initial conditions are not well known the use of either DNS or LES becomes problematical. Thus, from a viewpoint of desirability and cost effectiveness, RANS models will be with us for some time.

There are many forms that RANS models may take, especially when dealing with material mixing, at extremes or not. They vary from the most simplistic, where the flow is modeled as if it were a solid sphere moving through air, i.e., buoyancy–drag (Clift et al., 2005), to the two-fluid models where the key modeling term is the transfer mechanism of mass, momentum or energy (Youngs, 1989; Ishii and Hibiki, 2006). The individual fluids have as their derivation the Navier–Stokes equations. Another class of turbulence models (called that because they limit to single phase incompressible turbulence) start their derivation with the variable-density Navier–Stokes equations. Closure issues are the same as those for single-fluid incompressible flows (see for example, Chassaing et al., 2002). With additional complexity and uniqueness are multipoint models such as the spectral formulation of Steinkamp et al. (1999). Indeed, this later model is the only model (unless one thinks of DNS as also a model) that applies a consistent approach to all scales of motion; thus, for questions about the small scales due to reactions, etc., that information is available. Depending on the application (supernovae, ICF, large Mach number combustion) and the computational resources available, each of the above would have its advantages and disadvantages. Regardless of the path chosen, they are all well behind models for single-fluid incompressible turbulence.

4.3.5 Systematic Model Development and Assessment for Large Eddy Simulation (LES)

It is not feasible to compute large Reynolds number (Re) turbulent flows by directly resolving all scales of motion and material interfaces through *direct numerical simulation* (DNS); instead, macroscale portions of the unsteady turbulent motion are computed while the rest of the flow physics (including molecular diffusion and other microscale physics) remains unresolved. In *large-eddy simulation* (LES) (Sagaut, 2006; Grinstein et al., 2007), the large energy containing structures are resolved, and the smallest resolved scales are determined by the resolution cutoff prescribed by discretization or by a spatial-filtering process. In either case, unresolved structures are eliminated, and their effects on the resolved scales must be modeled. The Kolmogorov theory of turbulence provides a theoretical basis for models of such subgrid effects for equilibrium homogeneous isotropic turbulence (Lilly, 1964; Moser et al., 2009). In this special case, the critical interaction between resolved and subgrid turbulence is the exchange of energy. As a result, most subgrid model formulations are designed to be dissipative and act as a sink of turbulent kinetic energy, effectively regularizing the equations on the resolved scale. However, for turbulence that is strongly inhomogeneous, anisotropic, out of equilibrium, or that involves other physical phenomena that act at small scales, there is no theoretical basis for such subgrid models and the interaction between subgrid and resolved turbulence is more complex than simple exchange of energy. In such cases, LES modeling is presently primarily empirical.

A number of different formalisms and modeling approaches for LES have been proposed (Sagaut, 2006; Grinstein et al., 2007; Langford and Moser, 1999; Bazilevs et al., 2007), and a discussion of the conceptual issues surrounding LES is provided by Pope (2004). For the current discussion, we need only consider two general distinctions commonly made between the various LES approaches. The first distinction is between "continuous" and "discrete" LES. Continuous LES formulations define the simulated large scales through a continuous filter, so that the LES evolution equations are expressed as partial differential equations, with model terms to account for the subgrid effects. Discrete formulations either explicitly or implicitly define the large scale fields discretely, based on their numerical representation. The numerical solution of the LES equations for the former generally require that numerical resolution be significantly finer than the filter scale to eliminate significant numerical errors. However, this is rarely done in practice, which means that the numerical discretization and approximations are a nonnegligible part of defining the evolution of the large scales, effectively eliminating the distinction between continuous and discrete LES. The second distinction is between "explicit" and "implicit" LES modeling. In the former, explicit model terms describing subgrid effects are added, while implicit LES models use the dissipative nature of numerical approximations designed for shock-capturing and/or stabilization to regularize the equations (Grinstein et al., 2007; Bazilevs et al., 2007). The implicit LES approach based on shock-capturing is attractive in flows with strong shocks, where shock-capturing numerics are needed and can regularize the turbulence representation. However, as discussed above, in complex turbulent flows there are more subgrid effects than the energy transfer (dissipation) that numerical regularization or common explicit LES models are not designed to represent.

Even for turbulent flows of simple fluids, there is much room for improvement in the veracity and reliability of LES. LES of material mixing flows is particularly challenging: we must often

consider under-resolved material mixing promoted by an under-resolved velocity field and under-resolved initial conditions – which can be substantially more difficult. In many areas of interest such as inertial confinement fusion, the collapse of the outer cores of supernovas, and supersonic combustion engines, vorticity is introduced at material interfaces by acceleration or the impulsive loading of shock waves, and turbulence is generated via Rayleigh–Taylor and Richtmyer–Meshkov instabilities (e.g., Drikakis et al., 2005). In such flows, the basic physics of turbulent mixing is complicated by variable density, shock waves, and heat release from chemical or thermonuclear reactions. These complicating phenomena act at and affect the small scales of turbulence that are unresolved in LES, which, as discussed above, effectively invalidates the assumptions on which virtually all implicit or explicit LES models are based. Improving LES for such problems will require a focused research effort to formulate models that account for these complicating effects on the small scales of turbulence. Such an effort will necessarily be empirical, supported by extensive data on small-scale turbulence processes from both DNS and advanced experimental measurements.

Advances in LES for material mixing requires progress on modeling a number of processes occurring at small scales and their effects on resolved scale turbulence, including:

1. Baroclinic production of vorticity and other effects of small scale density variations.
2. Molecular scale mixing of species resulting in chemical or thermonuclear reactions and the resulting heat release.
3. Interaction of shocks and sharp material interfaces with turbulence.
4. Effects of unresolved (subgrid) perturbations on initial material interfaces.

In addition, the complexities of the material mixing problem will also likely require that two fundamental issues in the formulation of LES be addressed. First, in many (most) practical LES, the large scale turbulence that is being simulated is not precisely defined; that is, it is not generally specified how a turbulent field (e.g., from a DNS) would be processed to produce the corresponding large-scale field in the LES. In simple equilibrium turbulence, this does not cause a problem because the overall energy transfer from the resolved to subgrid scales does not depend on the details of this definition. However, with the complexities discussed above it is likely that the interaction between resolved and subgrid scales will depend on the precise definition of the large scales. Second, the purpose of an LES is to make inferences about the real turbulent flow of which it is a model. In simple turbulence, the quantities one wants to predict are dominated by the large scales (e.g., the turbulent kinetic energy), so evaluating them based on the resolved scales of an LES provides a good approximation of the actual quantity. However, in the complex turbulence characteristic of material mixing, one may be interested in quantities that are not so conveniently approximated in an LES, such as the degree of molecular mixing, the rate of reaction or even the vorticity statistics. In these cases, an auxiliary model of the contribution of unresolved scales to the quantities of interest will need to be formulated as part of an LES (Voelkl et al., 2000). See section 3.2.5 for additional discussion of some of the key theoretical issues associated with LES and subgrid-scale modeling.

A major research focus is on evaluating the extent to which particular subgrid physical effects can be implicitly modeled as the turbulent velocity fluctuations, recognizing when additional explicit models and/or numerical treatments are needed – and when so, addressing how to

ensure that the *mixed* explicit/implicit subgrid models act in collaborative rather than interfering fashion. An important challenge is to further understand the connections between implicit subgrid model and numerical schemes to reverse-engineer desirable subgrid physics; modified equation analysis provides a suitable framework in this context (Grinstein et al., 2007).

4.3.6 Systematic Model Development and Assessment with Direct Numerical Simulation (DNS)

Direct numerical simulation (DNS) of turbulent flows has played an important role in classical turbulence research, including the study turbulent mixing (Cabot and Cook, 2006; Livescu et al., 2009). The physical modeling issues associated with DNS are discussed in section 3.2.4. This is so primarily because the (usually incompressible) Navier–Stokes equations with Newtonian viscosity have been validated as a reliable model of many phenomena in simple fluids, including turbulence. As a consequence, accurate numerical solutions of the three-dimensional time-dependent Navier–Stokes equations for turbulent flows with particular initial and boundary conditions can be used as surrogates for physical experiments under the same conditions. Such numerical experiments have been scientifically useful because they allow precise control of initial and boundary conditions (Flores and Jimenez, 2006; Moser et al., 1998; Rogers and Moser, 1994), provide access to quantities that are difficult or impossible to measure (e.g., pressure–velocity correlations) (Hoyas and Jimenez, 2008; Mansour et al., 1988) and enable "experiments" that would be difficult or impossible to realize in the laboratory (Jimenez et al., 2004; Jimenez and Moin, 1991). However, to be used for predictions in particular flow configurations, DNS results must still be validated by comparison to experiments to ensure that models for the geometry, and initial and boundary conditions that are used to pose the DNS actually represent the flow situation of interest.

In material mixing flows, there are other important physical phenomena and associated models that are needed in a DNS, such as complex constitutive relations, chemical or thermonuclear reactions, thermodynamic equations of state, or interface mechanics. The models for these phenomena are often not as well validated as the Newtonian viscosity model for simple fluids. For this reason, use of DNS as surrogate experiments in such multiphysics flows is questionable (see section 3.2.4). However, DNS in such flows remains scientifically important for three primary reasons: first, it provides a good mechanism for testing multiphysics models in the absence of the large uncertainties introduced by RANS models or LES; second, multiphysics DNS can be used to evaluate turbulence models for use with the same multiphysics models used in the DNS; finally, it provides a mechanism for testing hypotheses about observed phenomena in multiphysics flows involving turbulence (Richardson et al., 2010). In this later scenario, a hypothesis about the primary cause of a phenomenon can be tested by posing a simple multiphysics model that should (under the hypothesis) exhibit the phenomenon and using DNS of the simple model to see if it in fact does. This approach has been used in classical turbulence (Jimenez and Pinelli, 1999).

To realize the benefits of DNS of material mixing, several ingredients are needed. First, the definition and role of DNS as described above must be clear. DNS is defined as the numerical solution of the equations of fluid mechanics with no turbulence models, along with models for any additional (multiphysics) phenomena, with sufficient resolution to represent all physical

time and length scales so that quantities of interest in the simulation have negligible numerical errors. Second, a systematic treatment of errors in DNS is needed. In DNS of classical turbulence, formal refinement studies have been performed (Donzis and Yeung, 2010; Donzis et al., 2008) and heuristics for resolution requirements have been developed. However, numerical error estimates are not generally provided for DNS and are needed (discussed in section 4.3.2). This is especially true in multiphysics flows, because the additional physics models can introduce new resolution requirements, which are not represented by the commonly used heuristics. Another source of uncertainty is statistical, arising from averaging over finite-sized samples. Estimates of such statistical errors are also needed (Jimenez and Moser, 2007). Finally, improved numerical/mathematical treatments of interfaces (immiscible fluids) and shocks are needed. Such discontinuities disrupt the resolution properties of numerical representations and can cause numerical error estimates to fail.

4.3.7 The "Material Mixing Transition", a Priority Grand Challenge

Material mixing to molecular scales as a consequence of stirring by turbulence is an important process in many practical applications and a significant aspect of most flows of interest to the DOE National Laboratories. In these flows, the various materials are not simply advected by the turbulence, since they actually set the physical properties of the mixture, may change phase, or undergo chemical or nuclear reactions. Thus, there is a strong nonlinear coupling between the mixing process and the underlying turbulence. To further compound the problem, the Schmidt and Reynolds numbers of the flows of interest are large enough so that only coarse mesh computations are feasible on today's supercomputers.

From the point of view of modeling the mixing process, both characterizing the mixing state and mixing rate are important. Depending on the specific problem, the mixing state can be described in sample space (e.g., Probability Density Function - PDF), scale (e.g., "blob" size distribution), or physical space (e.g., clustering). Mathematical tools are available for these descriptions, although in practice only low order approximations are used (e.g., the variance instead of the full PDF). Nevertheless, recent results show that, even for the simple case of homogeneous turbulent mixing between different density fluids, these are not enough to capture important physical effects (Livescu and Ristorcelli, 2008). However, data for constraining higher order quantities are difficult to obtain experimentally or accurately compute and, consequently, are scarce. The mixing rate is related to the accuracy of the physical model for mixing as well as to the coupling between the flow and the mixing process, and is far less understood. Again, data, either from physical experiments or DNS are needed to constraint or develop models. Since DNS potentially offers a wealth of information often inaccessible in physical experiments (Livescu and Ristorcelli, 2008; Rogers and Moser, 1994), albeit with severe restrictions with respect to the range of parameters accessible, it is especially important to assess the usefulness of such computations.

DNS is not feasible at the parameters found in the extreme applications of interest. However, one important idea has emerged, making fully resolved simulations at lower parameter values possible (Dimotakis, 2000). This idea is based on the experimental observation that turbulent flows undergo a "mixing transition", beyond which further increasing the range of scales (e.g., by increasing the Reynolds number) does not qualitatively change the mixing. For several

canonical flows this transition occurs at the same properly defined Reynolds number and it is hypothesized that all turbulent flows should undergo a similar transition. This is consistent with the current view on the transition to fully developed turbulence, when the flow restores all underlying statistical symmetries of the governing equations allowed by the boundary conditions (Frisch, 1996). Another possible interpretation of the "mixing transition" is related to the emergence of an inertial subrange in the turbulence spectra. Even though the "mixing transition" is supported both observationally and theoretically, some important questions remain before one can confidently scale numerical or experimental results to the extreme applications of interest:

1. Is there a "mixing transition" for complex flows and how should it be defined? For example, is the observed "mixing transition" described by the statistical restoration of symmetries? Or is it better to relate it to the emergence of an inertial subrange? If so, then how should it be defined in flows where the energy cascade is nonlocal?
2. Do the higher order quantities needed to describe the mixing undergo a "mixing transition" as well? If yes, at the same range of parameters as lower order quantities?
3. Can a universal value for properly defined parameters defining the "mixing transition" be found for complex flows?
4. Assuming a "mixing transition" always exists and can be quantitatively defined, how should the results be scaled to the extreme applications of interest?

Fortunately, it seems that on today's petascale computers accurate simulations of more complex flows are possible near the expected "mixing transition". The answers to the questions above may come from the simulations they are expected to support.

4.4 Crosscutting issues

4.4.1 Opportunities

The conduct of simulation depends greatly on the equations being solved; hence the activity of defining the models for turbulent mixing is extremely important. This is particularly important if the basic structure of the equations or models presently in use change. Similarly, the basic computational capability defines to some extent what constitutes a reasonable model. For example, exascale computing will allow consideration of intrinsically different modeling approaches where detailed constitutive calculations may be substituted for closed constitutive relations commonly used in simulations (see section 3.3.2). Another strong connection is the conduct of VVUQ, where the process of validation is fundamentally an examination of the fidelity of the model in a computational environment.

Experimental science impacts simulation principally through the VVUQ process. Validation treats observations or experimental data as the standard by which simulations are judged. Simulation also plays a key role in designing experiments and interpreting data. Furthermore, the ability to simulate an experiment should influence the development of experiments for the purpose of validation.

4.4.2 Goals for Short-, Intermediate-, and Long-Term Progress

As part of the identification of high-priority, high-impact research directions, goals for predictive simulation, VVUQ, systematic modeling, exascale computing and numerical methods

were established for short-term (1–5 years), intermediate-term (5–10 years), and long-term (10–15 years) progress.

1–5 year timeframe. The initial difficulty will be producing a coherent and focused effort toward the goals, given the breadth of challenges. The UQ methodology will need to be codified and begin to be applied to mixing. Simulations should achieve greater scalability and efficiency on modern computing architectures. The formalism for approximating interface dynamics will be improved.

5–10 year timeframe. The application of UQ methodology will be routinely utilized in simulations. We will achieve an understanding and appropriate treatments for interface initial conditions and the dependence of the solutions on them. Finally, we will be conducting a dedicated set of validations of simulations based on experiments designed specifically for that purpose.

10–15 year timeframe. We foresee having a modeling framework that understands and respects the physical nature of the material interface and the state of mixing.

5. Experiments and Diagnostics (K. Prestridge and J. Katz)

5.1 Summary

Current experimental capabilities can be partitioned into diagnostics, drivers, and data analysis. Details of current diagnostics capabilities are outlined in the next section. One of the key problems with Richtmyer–Meshkov and Rayleigh–Taylor material mixing experiments is that the acceleration profiles make it difficult to run statistically steady-state experiments and take data over long periods. For Rayleigh–Taylor mixing, the only steady-state data acquired thus far is from experiments performed in a water channel (Ramaprabhu and Andrews, 2004; Mueschke et al., 2006, 2009) and a gas channel (Banerjee and Andrews, 2006; Banerjee et al., 2010) at Texas A&M University. The presence of shocks in Richtmyer–Meshkov mixing experiments precludes steady-state measurements. There are several ideas in the Priority Research Directions section 5.3 below that discuss new drivers that will allow larger data sets. Larger sets of data help reduce statistical errors, and multiple forms of diagnostics on the same experiment can help better understand systematic errors for any given experimental configuration (a key component of the Material Mixing Olympiad described in section 3.3.4). A high priority for any new experimental work is very well characterized experimental error, emphasizing the possible sources of error. New experimental work must also characterize initial conditions as well as possible, due to the strong dependence of the subsequent flow on the initial conditions.

Rather than state Priority Research Directions we have chosen to capture the priorities via ten proposed experiments that demonstrate the directions and propose possible solutions. These experiments each seek to elucidate specific physics issues mentioned by the Theory/Modeling grand challenges and capability needs, while reflecting the accuracy and statistical requirements from the Predictions/Simulations considerations. One of the proposed research directions is in the area of high-energy-density (HED) diagnostic development. In our discussions, this area emerged as one in particular need of higher-resolution experimental

diagnostics, preferably leveraging the work done in low- energy-density flows; thus, an important consideration is that it is highly desirable for diagnostics developed at low energy, and/or single physics experiments to be extended to HED.

Before describing our ten priority research experiments, the next section presents a discussion of current diagnostic capabilities and future needs. This is intended to set-the-scene for the experiments, as an experiment without good diagnostics has no value.

5.2 Current Diagnostic Capabilities and Needs

General descriptions of the diagnostics available for fluid dynamics experiments are contained within the monograph by Tavoularis (2005). The following sections address the application of some relevant diagnostics to unsteady, high-speed, variable-density, and high-energy-density flows.

5.2.1 Particle-Image Velocimetry (PIV)

Particle-Image Velocimetry (PIV) measures the displacements of tracer particles to infer velocity (Adrian and Westerweel, 2010). The ability to measure two- and three-dimensional velocity measurements in a plane has been available for over a decade with high accuracy and resolution, and more recently techniques such as tomographic PIV enable three-dimensional velocity measurements in a volume (with approximately an order of magnitude inferior resolution). Typically, PIV is applied as an optical technique. However, the extension of PIV to extreme flows, in which optical access is not possible, is feasible using x-ray sources in either a scattering or absorption mode. An issue at extreme conditions is the (in)ability of particles to track the flow under very large accelerations. For recording high-speed flows, the advent of high-speed cameras and sources suggests that in about a decade, data rates of over 1 MHz may be readily accessible.

5.2.2 Coherent Anti-Stokes Raman Spectroscopy (CARS)

Coherent Anti-Stokes Raman Spectroscopy (CARS) is used for temperature and species concentration measurements (Begley et al., 1974; Tolles et al., 1977; Greenhalgh, 1987). Usually the measurements are so-called “point” measurements although there are a few recent demonstrations of line imaging measurements where laser sheets are crossed in a phase-matching scheme and an imaging spectrometer is used to detect the CARS spectrum as a function of distance along the line intersection of the laser sheets. The recent use of femtosecond lasers for CARS measurements has resulted in a two orders of magnitude increase in the data rate of the single-pulse measurements (Zheltikov, 2000). The main limitations of the technique in extreme regimes are due to the limited transmission of optical radiation in these regimes; even in cases where optical absorption is not an issue, there may be problems due to beam steering because of severe refractive index gradients. However, transmission and beam steering problems will be minimal if x-ray CARS can be implemented. X-ray CARS offers potentially much higher spatial resolution than optical CARS. The theory of x-ray CARS or x-ray stimulated Raman is not well developed; it is not possible at the present time to estimate what signal levels can be achieved with x-ray CARS.

5.2.3 Radiography

Radiographic techniques form an image of transmission using the contrast created by the interaction of particles (e.g., x-rays or protons) with matter (Barrett and Swindell, 1981). Typically, material density or areal density is inferred from the transmission field. A strength of radiographic techniques is that they are readily applicable in most extreme regimes; a weakness is that with a single-view measurement, radiography yields a measurement that is averaged in one direction (a line of sight measurement). To obtain three-dimensional reconstructions, 10–1000 views are typically required. The time resolution offered by radiography is already trending towards ~100 ns time between frames for specialized applications.

5.2.4 Laser-Induced Fluorescence (LIF)

Laser-induced fluorescence (LIF) is a technique extensively used to measure flow properties in complex reacting flows involving combustion, nonequilibrium chemistry, and plasma (Miles and Lempert, 1997). The technique involves using a laser to excite electrons into a state from which they decay with the release of a photon. LIF is typically implemented with visible and UV lasers and can provide quantitative data on concentration of species, temperature (translational, rotational, vibrational, electronic), pressure, and velocity under certain restricted conditions. Generally excellent temporal and spatial resolution can be obtained when pulsed lasers are used (tens of microns spatial resolution and sub-nanosecond temporal resolutions are readily achieved). X-ray fluorescence is an established technique for material analysis, but new x-ray laser sources could considerably improve the technique for extreme mixing applications. It may be possible to form the x-ray laser into a sheet to enable a planar measurement to be made of a particular species. Much research will need to be done to extend x-ray LIF to be more than a flow visualization technique. For example, a major difficulty will be to understand how the x-ray laser-induced fluorescence signal is affected by the local thermodynamic conditions and collisional environment.

5.2.5 Current High-Energy-Density (HED) Diagnostic Capabilities

While laser (OMEGA and NIF) and Z-pinch (Sandia Z) driven laboratory scale High Energy Density (HED) experiments are well developed, the available diagnostic capabilities are limited. In general, these experiments require diagnostics that operate in the x-ray spectrum to penetrate the common materials used in HED targets. Current capabilities in the x-ray regime include imaging (temporal resolution to 60 ps and frame rates of 16 GHz can be achieved), multi-monochromatic x-ray imaging (which provides multiple narrow spectral band images over a broad spectral range), x-ray Thompson scattering (which provides electron temperature and number density), neutron imaging, and gamma reaction history. Currently x-ray Thompson scattering and neutron imaging have limited temporal and spectral resolution. Gamma reaction history has excellent temporal resolution with limited spatial discrimination. VISAR (Velocity Interferometry System for any Reflector) can provide interface velocity. However, VISAR operates at optical wavelengths precluding its use for many HED experiments related to mix. For HED experiments to progress to the point that they can provide detailed data beyond mixing layer width will require significant advances in x-ray based diagnostics. Fortunately,

there is a path forward via the development of linear and nonlinear x-ray analogs of Raman and fluorescence techniques (see sections above).

5.2.6 Richtmyer–Meshkov Instability Investigation Utilizing Linear Stochastic Estimation (LSE)

The linear stochastic estimation (LSE) methodology (Adrian et al., 1989) was developed from Papoulis theory and is based on solving a multi-input/multi-output transfer function problem. It can be used with experimental, computational data or a combination of such data. For example, using a computational database to generate transfer functions and experiments as the input to the transfer function, LSE can assist in measuring turbulence statistics such as $\langle u'^2 \rangle$, $\langle \rho' u' \rangle$ and $\langle p' \nabla \cdot u' \rangle$ in large Mach number (~10) flows by not requiring each correlation to be acquired simultaneously. It can predict velocity and density separately using transfer functions and then correlate the predicted quantities.

LSE requires only one measured quantity to have temporal information. For example, high temporal resolution near-field pressure data can add temporal information to high spatial but low temporal resolution PIV data. Also, Computational Fluid Dynamics (CFD) can be used to form transfer functions that would expand the spatial and temporal resolution. LSE can be used with measurements other than just PIV and near-field pressure. Most new diagnostics, such as proton and x-ray radiography are limited in spatial or temporal resolution. LSE can provide means to compensate for one or the other. In many cases, experiments at large Mach numbers, reacting or ionized gas regimes are not accessible to diagnostics. LSE does not require the measurement to be in the flow field. Instead, transfer functions can be generated using CFD and then another quantity such as surface pressure can be measured to predict flow quantities within the flow field. LSE can also be used to provide time-resolved initial conditions for CFD analysis. This is often not available but is crucial for accurate predictions.

5.3 Priority Research Directions

5.3.1 Richtmyer–Meshkov Turbulence Statistics (see Appendix 10.1)

We must understand the parameters governing shock-driven, variable-density turbulent mixing through the measurement of turbulence quantities for Ma < 2, 0.5 < At < 1. Previous work in this area has provided insights into the initial condition dependence (Balakumar et al, 2008; Miles et al., 2005; Thornber et al., 2010), Atwood number effects (Weber et al., 2009; Motl et al., 2007; Jourdan and Houas, 2005) and Mach number effects (Leinov et al., 2009; Orlicz et al., 2009). However, there are no detailed measurements of turbulent fluctuations in this parameter space. These measurements will help elucidate the nature of unsteady, shock-driven, variable-density turbulent mixing, and how it compares with steady, isotropic, homogeneous flows upon which most turbulence theory and phenomenology are founded. It will also help understand the mixing transition as hypothesized and described by Dimotakis (2000) for unsteady flows and discussed in section 4.3.7.

Despite years of research, there are no reliable data on the turbulence properties of Richtmyer–Meshkov instability because of the difficulty in obtaining reproducible data sets that will include enough cases for a reliable statistical analysis. Even basic turbulence quantities such as Reynolds stresses (crucial for validation of turbulence models) are not available. Pulse

Detonation Engines (PDEs) provide the possibility to run repeatable consecutive tests at a rate that will allow collection of high quality data sets to provide reliable turbulence properties. The set up is simple and can become an excellent "canonical" test for validation of Richtmyer–Meshkov instability simulations. It requires a simple integration of existing test sections with the PDE or integration of PDE with buoyant jets, jets of various densities, and pulsed jets (Allgood et al., 2006; Kailasanath, 2003).

5.3.2 Chemistry Effects (see Appendix 10.2)

The experiments proposed here intend to study the effect of shock interaction with reacting flows that contain density gradients not aligned with the pressure gradient produced by the shock waves. The chemical reaction proposed here involves the production of a fine powder of titanium dioxide (TiO_2) resulting from the reaction of titanium tetrachloride ($TiCl_4$) and water (other similar reactions can be considered as well) (Hussain and Clark, 1981). The experiments will involve the effect of shock waves interacting with two gaseous fluids that are being mixed. One of the fluids will be tagged by $TiCl_4$ vapor while the other one will include water vapor. The mixing layer will be characterized by a cloud of TiO_2 powder that can be used as a seed for PIV measurements. The two-fluid mixing configurations can be one of several basic flows. In all cases, density gradients can be generated either by different gases or different temperatures and turbulence levels can be controlled:

1. Mixing layer: two adjacent fluids both in motion with different or equal velocities, one moving and the other at rest, or both at rest initially. The shock can be of different orientation relative to the boundary between the flows.
2. Jet stream into quiescent or moving flow (coaxial jet). The jet can be of different geometry and different orientation relative to the shock waves. In a coaxial configuration they can have different relative velocities. Variation on this configuration would be study of the interaction between multiple jets at different relative orientations, wall jets, impinging jets, etc.
3. Periodic ejection of jets, producing strong starting vortices to study interaction of shock waves with vortical flows, or alternatively, forced jets.
4. Coanda type flows can allow investigation of interaction of shocks with curved flows.
5. The above flow configurations can be accomplished also with liquid spray or mixing between liquid and gaseous fluids.

5.3.3 Interface Dynamics (see Appendix 10.3)

Experimental data to validate front-tracking algorithms are not widely available (these methods are discussed in section 4.3.1). In addition, Lagrangian tracking schemes fail upon merger of two or more large structures in instability-driven mixing flows. To improve the predictive capability and accuracy of such front-tracking schemes, a set of single-physics experiments are proposed that would study interface dynamics in turbulent mixing induced by Rayleigh–Taylor, Richtmyer–Meshkov, and Kelvin–Helmholtz instabilities. In addition, experiments quantifying de-mixing effects (Burrows et al., 1984; Smeeton and Youngs, 1987; Kucherenko et al., 1994) in Rayleigh–Taylor flow may also be used to enhance the validation envelope of such Lagrangian schemes. Existing experimental facilities at Texas A&M University, the University of Arizona (Waddell et al., 2001), the University of Wisconsin (Motl et al., 2009), Missouri S&T (Haley et al.,

2009), and Johns Hopkins University are proposed for this purpose. The facilities are all in the low-energy, large Schmidt number regime (i.e., cold experiments) and use immiscible/miscible fluid combinations. In addition, all experiments used for generating validation data sets must have controlled and quantifiable initial conditions for accurate comparison with numerical simulations and turbulence models. Diagnostics proposed include holography (for smallest scales); tomographic PIV with fluorescent particles, combined PIV/PLIF or combined hot/cold-wire anemometry, high-speed x-ray radiography for interface position and density statistics (for intermediate resolution), and; high-speed scanning laser sheets to measure interface position using fluorescent dye (at the largest scales).

5.3.4 Large Turbulent Mach Number Physics (see Appendix 10.4)

Experimental data on flows in which the turbulent fluctuations are compressible, meaning a Mach number of the fluctuations > 0.3, are not currently available. These data are of interest, because it is not clear what modifications need to be made to existing turbulence models to capture large Mach number effects. The physics at Ma ~ 10 involve ionization and disassociation, coupled with the possibility of "shocklets" that may substantially enhance the turbulence. In this sense, such behavior represents a true intermediate regime on the path to HED regimes, and an "additional physics" experiment. Due to these effects, optical diagnostics are not accessible, making the acquisition of correlations challenging.

5.3.5 High-Energy-Density Diagnostic Development

The high-energy-density regime, defined by the National Academy of Sciences Committee on High Energy Density Plasma Physics (2003), is energy densities > 10^{11} J/m^3 (or, equivalently, pressures > 1 Mbar), is ubiquitous to stellar objects, planetary cores, and inertial confinement fusion. Corresponding densities are generally on the order of solid density and above, and temperatures > 1 eV (~10^4 K). Mixing under these conditions is characterized by significant density differences and large mixing Reynolds numbers. Strong shocks, large accelerations, and large Mach number flow are also common. This configuration, along with the transient nature of many situations (ICF compression and thermonuclear burn occurs on time scales of nanoseconds and picoseconds, respectively) can lead to significant departures from mechanical (turbulent), thermal, and chemical/nuclear equilibrium. Diagnostics under these conditions are particularly challenging. Materials are generally opaque to optical wavelengths, thus necessitating the use of x-rays. The development of high brightness x-ray sources and associated diagnostic techniques has the potential to completely change the way in which laboratory high-energy-density experiments are conducted and the data that can be obtained. These techniques include linear and nonlinear Raman and other species-specific techniques, as well as techniques based on x-ray Thompson scattering and fluorescence. An example might be the x-ray analog of PIV that is specific to a particular species.

X-ray CARS or x-ray stimulated Raman spectroscopy are potentially powerful techniques for species and density measurements in HED media. X-ray Raman measurements of the C-atom have been demonstrated recently using 6.46 keV radiation from the Advanced Photon Source. The Raman scattering signature from the C-atoms was observed at a Raman shift of approximately 300 eV, with different structures in the Raman spectrum associated with different bonding states of the C-atom in different molecules or at different sites on the same

molecule. X-ray CARS has not yet been demonstrated, but planned x-ray Free Electron Laser (XFEL) sources should produce x-ray laser radiation with sufficient intensity and coherence to make such measurements feasible. A great advantage of x-ray CARS compared with x-ray absorption or fluorescence is that the x-ray wavelengths for the CARS experiments can be selected so that the medium has excellent transmission at these wavelengths. The XFEL must be capable of producing at least two different wavelengths so that the frequency difference of the laser beams can be tuned to the x-ray Raman resonances of the atomic species of interest.

5.3.6 Critical Schmidt Number for Immiscible Limit (see Appendix 10.5)

Material mixing is often partitioned into interpenetrating motions that "mix" the fluids and molecular diffusion. For two immiscible fluids, an interface separates the fluids and ensures that the fluids can only interpenetrate. However, for two miscible fluids there is the potential for both interpenetration and molecular diffusion. The Schmidt number measures the rate of momentum diffusion to mass diffusion, so that a small Schmidt number (of order one) means that mass and momentum diffuse at similar rates (e.g., in gases), where as in a large Schmidt number flow (e.g., immiscible fluids have infinite Schmidt number) the fluids purely interpenetrate. Thus, the question arises as to when increasing Schmidt number gives a flow a "mix" character that is better represented by two interpenetrating fluids (a so-called "two-fluid" model), rather than by a "diffusion" based model (e.g., gradient-transport). There are several important consequences to this question: in particular, if a numerical scheme is used to solve the governing equations then numerical diffusion could readily introduce unphysical mixing that might misrepresent what is essentially an interpenetration process between two fluids at large Schmidt number.

In an effort to investigate the effects of Schmidt number on Rayleigh–Taylor driven mixing, Mueschke et al. (2009) reported measurements of the molecular mixing fraction in a brine/water Rayleigh–Taylor unstable water channel. Their results indicate that for Schmidt numbers up to ~700, and for Reynolds numbers above 8000, the molecular mixing fraction is independent of the Schmidt number. This result is counter-intuitive for such a large Schmidt number and raises several questions, in particular: what is the relationship between Schmidt number and Reynolds number (for immiscible fluids there is no relationship that affects the molecular mixing fraction); do different flows exhibit the same result or are they fundamentally different; how does this result relate to the mixing transition (perhaps the transition needs refinement for material mixing applications); how are Schmidt number effects incorporated into mathematical models of mixing? The priority research direction then is to verify the results reported by Mueschke et al. (2009), and perform experiments at large Schmidt number (perhaps to 10000 – an "extreme" case) that can be used to verify and validate models of material mixing; these need not be Rayleigh–Taylor or Richtmyer–Meshkov instability experiments, and they might also be performed at high energy densities, or with widely differing material properties (perhaps the viscosity could be used instead of the mass diffusivity). The diagnostic grand challenge is to measure to the molecular level, and thus determine the fraction of molecular mixing in a highly turbulent flow.

5.3.7 Strength Experiment (see Appendix 10.6)

There is little research to investigate the effect of strength on turbulence. The report by Youngs (1997) suggests that strength serves as "drag" on the development of Rayleigh–Taylor and Richtmyer–Meshkov instabilities, and as a source of "dissipation" to the turbulent kinetic energy. Youngs includes two additional terms in his two-fluid model: a dissipation term for the turbulent kinetic energy and a momentum drag term, both with coefficients that need to be determined experimentally. The model suggests that the coefficients might be measured by determining the critical yield strength *Y* with different strength materials for fixed density difference and acceleration (or, fixing *Y* and choosing the acceleration to just overcome the strength). The materials to be used could be "jellies", which have previously been used to study Rayleigh–Taylor instability (Rogatchov et al., 1991; Meshkov et al., 2002). The dissipation constant might be measured from instantaneous velocity measurements (to obtain the turbulent kinetic energy), and release of potential energy requiring the measurement of density profiles (the difference is the dissipation, and from there the turbulent lengthscale may be inferred), necessitating the use of multi-probes.

5.3.8 Large, Sudden Energy Deposition into a Material

The goal of these experiments is to produce a first shock or reshock with different mechanisms for the shock; namely, the nearly instantaneous deposition of energy that will cause an interface to be unstable in the Richtmyer–Meshkov instability sense but from a different mechanism. One possibility is energy deposition from a proton radiography source into one material that would be opaque, and the other being invisible to the pRad beam. The desired measurements are of mean and fluctuating density and velocity fields.

5.3.9 Turbulent, Shock-Compressed, Particle-Laden Flow (see Appendix 10.7)

Flow and transport phenomena associated with interaction of a particle field with shock waves in the 1.1–15 Mach number range introduces a particularly challenging modeling problem, for which there is presently very little experimental data. The particle field could represent, e.g., suspended sand or a cloud of droplets entrained from a liquid–air interface, and they would range in size from microns to millimeters and in density from 800 (oil droplets) to 2500 kg/m^3 (sand). The associated relaxation times of the particles in response to the change in velocity across the shock would vary from microseconds to milliseconds, which would result in very different dispersion rates. Obtaining quantitative data in such an environment is a major challenge, and should include the flow of the continuous phase along with the relative motion of the dispersed particles. In dilute suspensions, PIV can be used for mapping the gas flow (with seed < 0.1 m seed particles), and various tracking technique can be utilized for measuring the particle motion. Phases can be distinguished based on particle size or using fluorescent particles (either as tracers or dispersed phase) that respond at a different wavelength to an illuminated laser, i.e., PLIF based techniques. High-speed digital holography and/or tomographic PIV could be used for three-dimensional tracking of the particle field and ambient flow. Lagrangian autocorrelations of the particle trajectories could be used for efficiently determining the diffusion coefficients of the dispersing cloud, thus providing critical data for numerical modeling of such flows.

In dense suspensions, the medium becomes opaque, requiring development of new measurement techniques for mapping the spatial distribution of the particle field. In the near term, x-ray imaging could be used for obtaining the global properties of the suspension, such as boundaries and semi-quantitative spatial distribution based, e.g., the distribution of density in x-ray images. Multi-view x-ray imaging could be used for mapping the global properties of the suspension. In the case of suspended droplets, in the near future, inserted optical probes could also be used for obtaining statistics on the flow and particles at selected points. Micro LDV probes could measure the airflow, and fiber optic probes could provide a time series of data on the size and concentration of droplets passing through the probe. However, the latter would introduce considerable uncertainty. In the 5–10 year span, the introduction/availability of coherent x-ray sources would allow the possibility of recording x-ray holograms. When combined with microscopy, which would require development of appropriate refractive elements (some are already available), it would be possible to measure the spatial distribution of particles in dense suspensions. Furthermore, x-ray microscopic holography would facilitate measurement of three-dimensional crystal structure within materials.

5.3.10 Multiphysics Statistically Steady Turbulence (see Appendix 10.8)

Shock tubes provide our most powerful tool for investigating Richtmyer–Meshkov instability since the initial conditions are well defined and relevant parameters can be varied over a wide range. A major limitation of shock tubes, however, is that the amount of data that can be extracted from them is relatively low. The low data rate becomes particularly problematic for the validation of models used in RANS and LES codes since well-converged statistics of velocity and scalar fluctuations are required. For example, turbulence model validation may require converged probability density functions of velocity and scalar fluctuations, and their correlations, such as Reynolds stresses and turbulent scalar fluxes. It can take several thousand data points to achieve sufficiently converged statistics of these quantities. For this reason it is desirable to consider new methods for studying the Richtmyer–Meshkov instability that may enable significantly larger data sets to be acquired. One possibility is to use a steady supersonic wind tunnel flow to generate a statistically-stationary unstable/turbulent flow that is sustained by a shock impinging on an interface with a density gradient.

5.4 Cross-Cutting Issues

Several cross-cutting issues emerged from the experimental priorities. These focus on the reproducibility and repeatability of experiments, diagnostic resolution, experimental error estimates, and known and well-characterized initial conditions. The first two issues inform the error estimates. While individual experimental results are often published, the accompanying results often have error analysis for one set of experiments. Very rarely are statistical ensembles of data acquired so that variance in the results can be understood. Also very rarely are multiple diagnostics used to make the same measurement simultaneously on one experiment to check accuracy.

Understanding diagnostic measurement error and its relationship to large or small ensembles of data should be emphasized in future experimental work, and these results should be communicated together with the data. The measurement error also must be incorporated into the presentation of initial conditions. Since the experimental initial conditions must be used to

initialize simulations and RANS models, they should be as well resolved as possible. The goal of characterizing the initial conditions should be to understand as well as possible the role of noise on the flow development, and possibly the amplitude and frequency spectrum of possible noise in the experiment. Due to difficulties in making measurements of noise that are within the same noise range as many common experimental diagnostics, new ideas on how to best constrain the initial conditions will have to be explored with the simulation community.

New developments in diagnostics are required to take us to more extreme flow conditions. Understanding material mixing requires measurements of scalar and vector quantities at the smallest energy-containing scales of mixing. These measurements become more difficult as the speed, temperature, and energy-density of the flow increases. The experimental priority research directions provide guidance on the key physics areas where we can advance physics understanding through diagnostic development and new experiment development. Short-term work in the next 5 years will leverage our current capabilities to collect turbulent cross-correlation terms in moderate flow conditions. New experimental capabilities will leverage this work out in the next 10 years to flow conditions that address specific physics concerns, such as multiphase and reacting flows. Long-range plans include developing diagnostics for HED flows that will allow us to penetrate the mixing regions with greater resolution than ever before achieved, while developing drivers that will get us to new regimes while still allowing repeatable, frequent experiments for the collection of statistical data.

6. Conclusions

The breadth and extent of this report indicate the opportunities and challenges that reside with material mixing. The extensive set of proposed experiments reflects the set of theory/modeling challenges, and the requirement on experiments for high fidelity diagnostics is well prioritized by the predictions/simulations. The last 15 years has seen a ten-fold increase in diagnostic capability, computational speed, and understanding of material mixing models and their development. There is no reason to believe that the next 15 years will be any different, but with new sets of challenges and opportunities. There are clearly several themes throughout the discussions in this report:

1. The need for high fidelity diagnostics and associated measurements for parameters relevant to advanced theories and models, and for VVUQ. Conversely, theories must be aware of experimental and diagnostic restrictions (e.g., sometimes simpler theories are better).
2. The role of "reaction" in material mixing is clearly an open question across all focus areas – the theory is difficult and complex, the simulations lack resolution, the models need major refinement, and the experiments need substantial diagnostic development.
3. A unique aspect of fluid mixing, when compared with other physics problems, is the role of statistical models; inherently mathematical descriptions of turbulence are statistical, but the collection of statistical data in extreme flows, or from simulations, necessitates either statistically steady experiments, or extensive sets of statistically related experiments.
4. It is evident that the presence of shocks cross-cuts difficulties with material mixing theories, the need for advanced numerical methods, and experimental diagnostics. It seems likely that shocks will continue to represent one of the grand challenges for material mixing into the foreseeable future.

It is evident that research for material mixing at extremes demands collaboration between disparate expertise (it seems unlikely that a single person can realistically master all the associated fields of theory, simulation, and experiment) but, more than that, a strong element of co-design is needed that this report has tried to capture. To this end the priority of a Material Mixing Olympiad is perhaps one integrating theme, and another is the formation of the CoMuEx at LANL. A third is the formulation of a decadal study that focuses on the need for co-design in material mixing at extremes. All three should proceed in parallel with support from new diagnostic facilities such as MaRIE, and appropriate long-term funding.

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8. Appendix A – Participants

Assignments and Questions: 1/7/2011

Research Needs for Material Mixing at Extremes

Contact: Malcolm J. Andrews, 505-606-1430, mandrews@lanl.gov

Assignments and Questions for Theory/Modeling

Snezhana Abarzhi Malcolm Andrews Cris Barnes Timothy Clark Sharath Girimaji Robert Gore Jeffrey Greenough Sanjiva Lele Len Margolin Dale Pullin Raymond Ristorcelli Robert Rubenstein Oleg Schilling David Sharp Krista Stalsberg-Zarling Robin Williams	1. How "predictive" are we? How is "predictive" defined? 2. Are there examples of classical modeling approaches that fail in extreme conditions (e.g. gradient-diffusion), and perhaps not even capable of mimicking the physics (i.e. needs more than resetting a "constant")? What is the role of stochastic (e.g. probability density function) approaches? 3. In RANS approaches is it preferable to have fewer model equations with better submodels or to have more model equations with "less modeling" in each? 4. Any reason to believe that the paradigm of RANS for complex flows, LES for in between and DNS for simple will not hold into the future with just different definitions of simple, complex and in between? 5. Will experiments, modeling and DNS converge at some point – what are the blocks (e.g. initial/boundary conditions, numerical methods, modeling approaches, experimental measurements, fundamental equations, metrics, theory)? a. What does DNS with strong shocks mean; what does DNS with surface tension or strength in one material mean; what does DNS with strength mean since plasticity is a phenomenological model? b. What is the basis for DNS with reactions, i.e. does Newtonian viscosity hold when there are reactions that cause volumetric heating and products at different energies and mean free paths? c. What does Fickian diffusion mean and does it apply? d. Equation-of-State (EOS) of mixtures under extreme conditions for DNS? e. Is it wise to use DNS as a surrogate for experimental data? Under what conditions is this valid? The implications are profound. Experiments are the avenue to discovery, if DNS is not a surrogate for experiments it should not be used for discovery either.

Assignments and Questions for Predictions/Simulations

Mark Chadwick James Fincke Cris Fryer	1. What will we really be able to do with exascale? 2. What will the framework for combining simulation, and experimental uncertainties look like? Will methods for computing start to embed the methodology for uncertainty? I.e., polynomial chaos, adjoints, etc. 3. VVUQ (i.e. Verification, validation and uncertainty quantification) of

Fernando Grinstein James Kamm Robert Little Daniel Livescu Robert Moser William Rider Kimberly Scott Michael Steinkamp	simulated effects of near-interface dynamics (interface treatments): what test cases, experiments, metrics? Generally, the mathematical theory for simulation of interfaces is lacking, i.e., convergence, entropy conditions. The question of mathematical theory for the convergence of numerical methods for interface is in need of development. 4. What will predictive software look like. Will we be able to program or perhaps we shall live in Matlab like worlds? What role will visualization play? 5. Are we looking at the right metric for mixing now (i.e. vorticity), and how does this change with physical complexity associated with extremes (shocks, radiation, magnetics, relativistic effects.).

Assignments and Questions for Experiments/Diagnostics

Kathleen Alexander Arindam Banerjee Robert Benjamin Riccardo Bonazza William Buttler Noel Clemens Michael Dunne Ephraim Gutmark Jeffrey Jacobs Farzaneh Jebrail Joseph Katz Carolyn Kuranz Robert Lucht Katherine Prestridge Devesh Ranjan Christopher Tomkins Jonathan Workman	1. How and how well can we measure statistical quantities such as $\langle u'^2 \rangle$, $\langle \rho' u' \rangle$ and $\langle p' \nabla \cdot u' \rangle$ in: large Ma (~10) Richtmery–Meshkov; in gas–solid turbulent flows; any HEDP with reaction flow, any HEDP experiment? 2. What spatial and temporal resolutions can we achieve density, velocity, temperature? 3. Can we list new diagnostic techniques that we would like to develop (i.e. not incremental improvements to PIV), and e.g. what can we achieve with radiography—proton, x-ray, or other—in terms of fluid mechanical measurements as these might become more and more relevant with very large Ma? 4. What types of experiments can be developed to make the large Mach number, or reacting, or ionized gas regimes more accessible to diagnostics? 5. Where do we accept a compromise (quality, amount, cost) for data at extremes?

Agenda

9. Appendix B - Agenda

Research Needs for Material Mixing at Extremes

January 9 to 12, 2011
La Fonda Hotel, Santa Fe NM

Sunday, January 9, 2011

5:30-7:00 PM **Registration (just behind the ground floor restaurant)**

Monday, January 10, 2011

Welcome
New Mexico Room

7:45 AM	**Continental Breakfast/Registration**	
8:15 AM	**Welcome**	John L. Sarrao
8:20 AM	**Workshop Overview and Charge**	Malcolm Andrews

Plenary Session – Research Grand Challenges for Material Mixing at Extremes
New Mexico Room

8:40 AM	**MaRIE Overview** *Cris Barnes*
9:00 AM	**Fluid instabilities and Mixing in Extreme Conditions** *Oleg Schilling/Rob Gore*
9:40 AM	**Material Mixing at High Energy Density** *Jim Fincke/Malcolm Andrews*
10:20 AM	**Coffee break - discussion**

10:50 AM **Mixing in Astrophysics**
Chris Fryer/Robin Williams

Overview of Panel Structure/Vision - Panel Leads (in pairs)

11:30 AM	Experiments/Diagnostics	Kathy Prestridge/Joe Katz
11:45 AM	Theory/Modeling	Oleg Schilling/Dale Pullin
12:00 PM	Simulations/Predictions	Fernando Grinstein/Bill
	Rider	

12:15 PM **Lunch – Santa Fe Room**

Breakout Session #1 (3 parallel rooms)- Panel Discussions

1:45 PM **Initial Panel Breakout Discussions**

Experiments/Diagnostics	*Location - New Mexico Room*
Theory/Modeling	*Location - Santa Fe Room*
Simulation/Predictions	*Location - Coronado Room*

(Optional presentation of participant response to 1 question with 1 slide)

3:30 PM **Coffee break - discussion**

4:00PM **Continue breakout panel discussions and generate first round of synthesis**

5:30PM **End of Day One Deliberations**

5:30 pm **Panel Chairs meeting – status/issues/info for next morning**

6:00 PM **Social hour at La Terraza + cash bar**

7:00 PM **Banquet - La Terraza - Keynote Speaker: Michael Dunne ("*Why controlling mix could enable LIFE*")**

Tuesday, January 11, 2011

8:00 AM **Continental Breakfast**

Breakout Session #2 (3 parallel rooms)- Distillation of Panel Input

8:30 AM **Continue Breakout Discussions in 3 panel rooms – based on answers to questions the drafting of *priority research directions*, *capability opportunities*, and *projected capability needs***
Same rooms as Monday afternoon breakout session #1

10:00 AM **Coffee break - discussion**

10:15 AM	**Plenary Session in New Mexico Room – Panel Reports**	
	Initial panel output highlighting ***draft priority research directions and capability gaps*** (each with 20 minute presentation + 20 minute discussion)	Panel Leads
	Experiments/Diagnostics	*Kathy Prestridge/Joe Katz*
	Theory/Modeling	*Oleg Schilling/Dale Pullin*
	Simulations/Predictions	*Fernando Grinstein/Bill Rider*
12:15 PM	**Lunch – Santa Fe Room**	

Plenary Session: Grand Challenge Cross-Cutting Capability Needs
New Mexico Room

1:45 – 3:30 PM	**Cross-Cutting Needs/Next Steps/Priorities**	Malcolm Andrews
3:30 PM	**Coffee break**	
4:00 PM	**Plenary session continues - Cross-Cutting Discussion**	Malcolm Andrews
~5:30-8:00 PM	**Executive Committee Meeting (all are welcome)**	

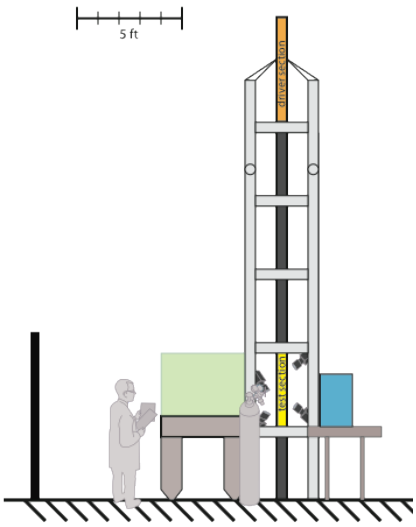
Wednesday, January 12, 2011

8:00 AM	**Continental Breakfast**	
8:30-12:00PM	**Final report, discussion and plans**	Malcolm Andrews
12:00-1:30PM	**Lunch –Santa Fe Room**	
1:30PM-4PM	**Open meeting of Organizing Committee for writing**	Malcolm Andrews

10. Appendix C- Details on Experiments

10.1 Richtmyer–Meshkov Turbulence Statistics

A shock-tube optical diagnostic experiment that might operate to Ma ~ 6 and employs PIV and LIF to simultaneously probe the mixing volume has the advantage of building on current advanced diagnostics that we might reasonably expect to improve over the next 15 years, using known technologies to build and validate a new facility (this could take 10 years), and be substantially less expensive than an explosively-driven experiment.



Another simple driver that would allow more experiments, and therefore more data, is a pulse detonation engine (PDE) that produces a sequence of high-speed shock waves (Mach numbers on the order of 10) at rates of up to 100 per second. A tube is periodically filled with a reactive gas mixture, a detonation is initiated at the back end, the detonation wave propagates through the tube, and the product gases are exhausted through the front end. The tube is scalable in a wide range of sizes (length and diameter), can have different cross-sectional geometry, shock wave speed can be controlled by changing fuel, equivalence ratio, or tube fill fraction as well as their rate. Experimental arrangements used to study Richtmyer–Meshkov instability (such as shock tubes) could be easily modified for use with PDEs by substituting PDE for the Driver and Diaphragm section. Air from PDE can be utilized as half of fluid interface or it is possible to inject another shock carrying gas. Dense gas such as SF_6 or lighter gas such as Helium could be used as gas injected from opposite direction. Perturbations will occur naturally from noise caused by a deflagration-to-detonation transition (DDT) device and injection mechanism. The advantages of using the PDE include:

1. Reproducible shock waves at rates that allow repeatable measurements necessary to achieve statistically significant turbulence properties not available otherwise.
2. Arrays of PDEs can be used for circumferential formation of converging shock waves.
3. IC and BC can be accurately measured.
4. Can be used for gas–gas, gas–liquid, and gas–solid interfaces.

5. Diagnostics exist to obtain the necessary turbulence and mixing properties.
6. Wide range of high strength shock waves is available.
7. Rapid turnaround in experimental configuration.
8. Naturally occuring initial perturbation due to fill cycle.
9. Test Richtmyer–Meshkov instability in a realistic setup.
10. Scalable in a wide range of sizes (length and diameter), can have different cross-sectional geometry.

The pulsed detonation actuator to be used in this investigation consists of a tube closed at one end and exhausting into the test section at the other end. The cross-sectional geometry of the pipe, its diameter and length can be adapted to the particular test set-up. Fuel and oxidizer are injected into the tube and mixed. Once the desired fill fraction is achieved (defined as the volume of the tube filled with combustible mixture divided by the overall volume of the tube) a spark ignites the mixture and a deflagration wave begins to propagate, transitioning into a detonation wave by deflagration-to-detonation transition (DDT), at which point the shock wave propagates towards the test section at speed of 3 km/sec, or Ma = 6–8. This process can be repeated at rates of up to 100 Hz. Detonation has an associated lower entropy production compared to deflagration, and therefore is theoretically a more efficient means of converting the stored chemical energy.

10.2 Chemistry Effects, not Classical Combustion

There are several laser-based diagnostic techniques that can be applied to quantify the flow characteristics of the experiments proposed in 5.3.2.

1. **Spectrally resolved absorption**. The absorption measurements utilize tunable diode lasers (TDLs) as light sources. They can be used to acquire time-resolved measurements of velocity, temperature, and species concentrations. Their limitation is that they provide line of sight integrated data.

2. **Planar laser-induced fluorescence (PLIF) imaging**. PLIF provides the spatially resolved planar distribution of the reactants and the product species, temperature measurements in air flows using acetone seeding, and mixing layer visualizations.

3. **Molecular Rayleigh scattering**. Rayleigh scattering can be used to determine flow field, density, and in some cases temperature when the pressure is known, and mixture fraction.

4. **Raman Scattering**. This technique provides single-shot spatially-resolved multiscalar measurements of species concentration and temperature in turbulent reacting flows.

5. **Particle image velocimetry** (**PIV**) is a laser-based method for acquiring spatially resolved planar turbulent flow measurements. It is used to obtain instantaneous and mean velocity measurements. Recently, PIV systems can yield relatively high temporally resolved flow field information.

6. **Laser Doppler velocimetry (LDV)**, or laser **Doppler anemometry (LDA)** is a technique for measuring velocity vectors of flows. It provides specially and temporally resolved flow information at a particular point in the flow field.

10.3 Interface Dynamics

The need is to have single-physics experiments that would provide high fidelity datasets of three-dimensional velocity and density statistics to quantify interface dynamics in Rayleigh–Taylor and Richtmyer–Meshkov instability driven flows. The datasets will then be used to validate front-tracking algorithms used in Lagrangian codes.

Regime of the flow:

Rayleigh–Taylor: Re > 10000, At = 0.1–0.9, accelerations 1g–60g

Richtmyer–Meshkov: Re > 100000, At = 0.1–0.95, Ma up to 2.5

Rayleigh–Taylor De-mixing: Re > 10000, At = 0.1–0.5

10.3.1 Diagnostics Available and Possible Future Ones

Rayleigh–Taylor: Imaging, PIV/PLIF, thermal anemometry, pH indicator-based diagnostics, x-ray radiography (the facility at the University of Wisconsin currently uses high speed x-ray radiography at ~250 fps sampling rate). Future plans involve increasing the sampling rate and extracting density spectra by incorporating higher performance, structured scintillator screens, higher resolution/gain image intensifiers and a higher power x-ray source).

Richtmyer–Meshkov: PIV/PLIF, Planar Mie Scattering, Rayleigh Scattering

Rayleigh–Taylor De-mixing: Imaging, PIV/PLIF, pH indicator based diagnostics

10.3.2 Critical Parameters to Measure, any Dimensionless Numbers, etc.

Rayleigh–Taylor: mixing layer widths, growth constants, density–velocity correlations, b, a, θ, higher order statistics, PDFs, single-mode terminal velocities and Froude number.

Richtmyer–Meshkov: mixing layer widths, growth constants, circulation, density–velocity correlations, b, a, θ, higher order statistics, PDFs.

Rayleigh–Taylor De-mixing: mixing layer widths, growth constants, density–velocity correlations, b, a, θ, higher order statistics, PDFs.

10.4 Large Turbulent Mach Number Physics

The need is sufficient fidelity to obtain simultaneous three-dimensional velocity and scalar fields in flows with significant compressibility effects in the fluctuations. Such data would provide validation of existing models, and likely modification of those models to incorporate new physics and mixing mechanisms.

We can build upon current advanced diagnostics that we might reasonably expect to improve over the next 15 years, using known technologies to build and validate a new facility (this could take 10 years). Diagnostic improvements include multiple axes for three-dimensional measurements; higher spatial and time resolutions (to obtain molecular mixing measurements); and, introduction of multiprobe techniques to obtain PIV type measurements of velocity fields.

Based on a Ma ~ 15 shock interacting with a He/Xe interface and using normal shock relations, we can roughly estimate the following parameters (based on an integral mixing lengthscale of 1 cm, and properties of He/Xe):

Turbulent fluctuation velocities ~ 850 m/s

Bulk Reynolds number ~ 770000

Fluctuation Reynolds number ~ 150000

Kolmogorov scale ~ 1.28 μm

Taylor scale ~ 1.0 mm

Eddy turnover time ~ 0.03 μs

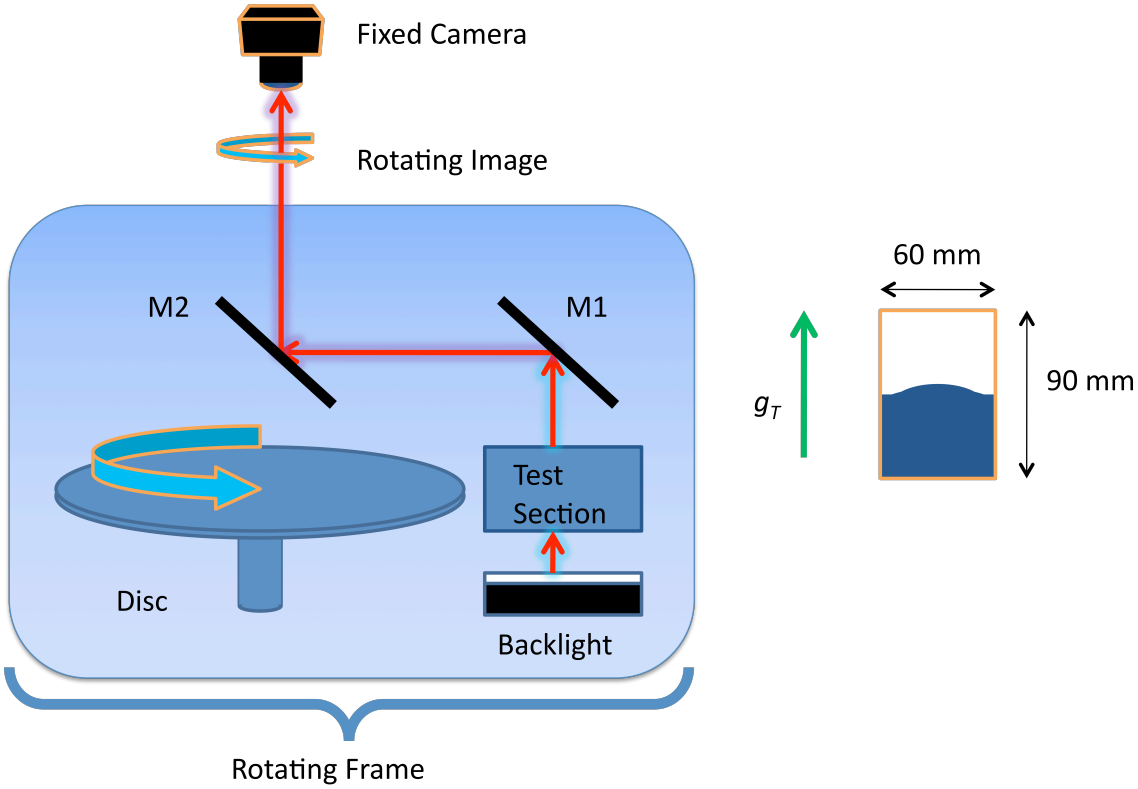
To resolve the eddy flow field would require a time resolution less than 0.03 μs, but not "sequential" images at that time spacing.

10.5 Critical Schmidt Number for Immiscible Limit

At a Schmidt number of 1 significant molecular mixing is known to exist in Rayleigh–Taylor driven turbulence (Ramaprabhu and Andrews, 2004). Moreover, Mueschke et al. (2009) determined that for Schmidt numbers up to 700 and Reynolds numbers above 10000 the molecular mixing was still similar to the Sc ~ 1 result. However, it is evident that for infinite Schmidt number (immiscible fluids) the molecular mixing must be zero. It is an outstanding question to determine at what Schmidt number molecular mixing is constrained. The idea here might be to use larger Schmidt number fluids in a facility similar (but bigger) to that of Mueschke et al. (2009). The large facility would enable larger Reynolds numbers, but may need to be four times larger to realize large enough Reynolds numbers to be conclusive. Very large Schmidt numbers (~10000) experiments might also provide useful validation date for interface tracking algorithms.

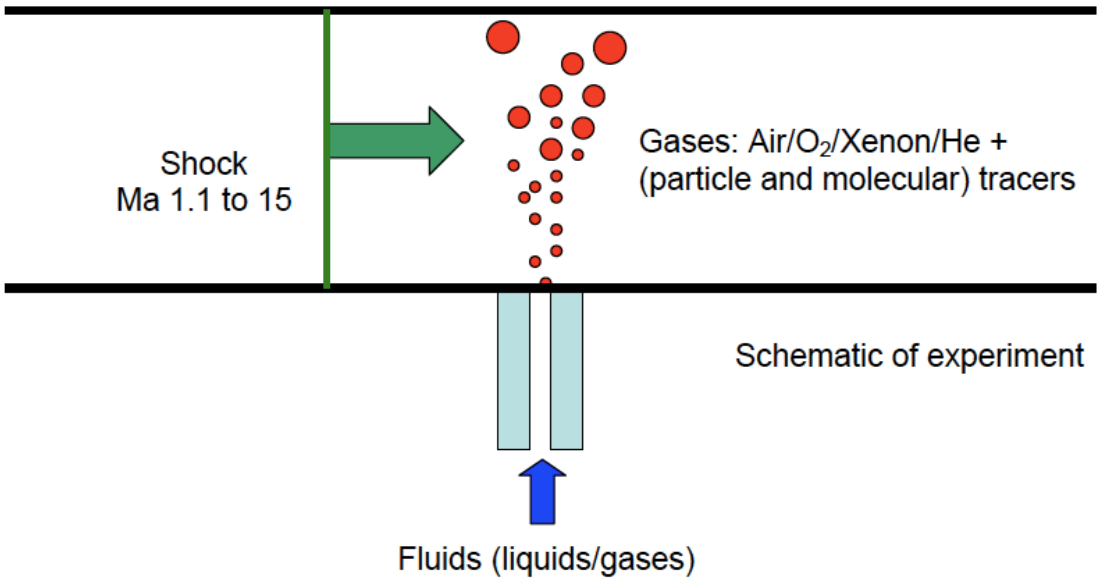
10.6 Strength

An example of strength experiments is the use of mayonnaise to set up an interface. The precise control one has over the interface is an advantage. Also, with the rotating experiment, below, the experiment can be run at 100 rpm, and a high-speed camera used to capture the movement of the interface.



10.7 Turbulent, Shock-Compressed, Particle-Laden Flow

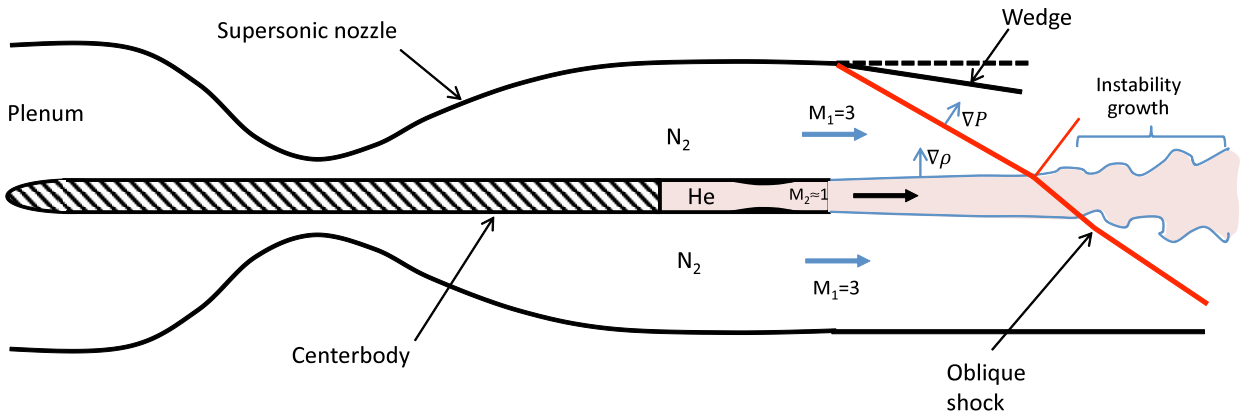
One possible experiment is a shock accelerated particle-laden flow. The shock can be driven by a tube, or with a PDE, as mentioned in section 10.1. The particle-laden flow can be variable density, buoyant, turbulent, or laminar, and the nature of the particles could be varied such that they were all of the same diameter, or a known distribution of particle sizes was used.



10.8 Multiphysics Statistically Steady Turbulence

One possibility is to use a steady supersonic wind tunnel flow to generate a statistically stationary unstable/turbulent flow that is sustained by a shock impinging on an interface with a density gradient. For example, consider the configuration below that shows a Mach 3 wind tunnel with a centerbody separating the supersonic flow into two sections. The centerbody is a plate and so the resulting flow is two-dimensional (in the mean). The centerbody contains another nozzle that could have a lower Mach number than the outer flow. This inner nozzle could flow a gas with a lower molecular weight to produce the desired density gradient. For example, if the Mach 3 flow is N_2 and the centerbody flow is Helium with near unity Mach number, then the velocities of the two streams will be approximately matched. In this case, the coflowing streams will exhibit density stratification and the flow will be essentially shearless. Owing to the low shear the flow will remain laminar for a considerable distance downstream provided the Reynolds number remains small enough. If a wedge is placed on the upper wall, an oblique shock can be made to impinge on the density interface. The resulting misalignment of the density and pressure gradients (see figure) will induce baroclinic vorticity. The resulting instability will grow in space and time as the flow advects downstream. The magnitude of the induced baroclinic torques can be varied by changing the molecular weights and temperatures of the gases, or by changing the shock strength. Since the acoustic impedance will likely not be matched across the density interface, there will be a partial reflection of the shock from the interface.

Since this flow can be setup in a continuous or quasi-continuous wind tunnel, it is possible to use conventional laser diagnostic techniques to obtain datasets composing thousands of images. For example, Mach 3 flows are relatively straightforward to seed with a fine aerosol (such as mineral oil from a smoke machine or TiO_2 from a fluidized bed) to enable PIV measurements to be made. Furthermore, the jet flow can be seeded with a fluorescent tracer such as NO to enable helium concentration measurements to be made with the PLIF technique. If NO is seeded into both the outer and inner flows then a two-line fluorescence measurement enables the instantaneous temperature to be inferred. Simultaneous concentration–velocity or temperature–velocity measurements will enable the computation of the correlations needed for validation purposes.



Schematic diagram of the setup that could be used to study Richtmyer–Meshkov instability in a statistically stationary flow.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